FULL SEARCH HISTORY

```
=> d his nofile

     (FILE 'HOME' ENTERED AT 15:05:43 ON 03 JAN 2008)

     FILE 'HCAPLUS' ENTERED AT 15:05:55 ON 03 JAN 2008
                E US20070128704/PN
L1              1 SEA ABB=ON  PLU=ON  US20070128704/PN
                D ALL
                SEL RN

     FILE 'REGISTRY' ENTERED AT 15:07:39 ON 03 JAN 2008
L2             13 SEA ABB=ON  PLU=ON  (108-30-5/BI OR 108-32-7/BI OR
                   116539-55-0/BI OR 142-82-5/BI OR 164071-56-1/BI OR
                   16940-66-2/BI OR 23229-69-8/BI OR 260354-12-9/BI OR
                   40570-64-7/BI OR 74-89-5/BI OR 861995-99-5/BI OR
                   9001-62-1/BI OR 96-49-1/BI)
                D SCAN
L3              6 SEA ABB=ON  PLU=ON  L2 AND 1/S
                D SCAN
L4              7 SEA ABB=ON  PLU=ON  L2 NOT L3
                D SCAN
                D L3 1-6
L5              1 SEA ABB=ON  PLU=ON  40570-64-7/RN
                D SCAN
L6              1 SEA ABB=ON  PLU=ON  116539-55-0/RN
                D SCAN
L7              1 SEA ABB=ON  PLU=ON  260354-12-9/RN
                D SCAN

     FILE 'STNGUIDE' ENTERED AT 15:15:25 ON 03 JAN 2008

     FILE 'REGISTRY' ENTERED AT 15:17:42 ON 03 JAN 2008
                D SCAN
L8              1 SEA ABB=ON  PLU=ON  164071-56-1/RN
L9              1 SEA ABB=ON  PLU=ON  861995-99-5/RN
L10             1 SEA ABB=ON  PLU=ON  L2 AND C4 H4 O3/MF
                D
L11             1 SEA ABB=ON  PLU=ON  108-30-5/RN
                D SCAN L4
L12             1 SEA ABB=ON  PLU=ON  METHANAMINE/CN
                D RN
L13             1 SEA ABB=ON  PLU=ON  L2 AND LIPASE
                D CN
                D RN
L14             1 SEA ABB=ON  PLU=ON  9001-62-1/RN

     FILE 'HCAPLUS' ENTERED AT 15:30:40 ON 03 JAN 2008
                D SCAN L1

     FILE 'CASREACT' ENTERED AT 15:31:03 ON 03 JAN 2008
L15             6 SEA ABB=ON  PLU=ON  L5/RCT(L)L6/PRO
                D SCAN
L16             4 SEA ABB=ON  PLU=ON  L5/RCT(L)L7/PRO
                D SCAN
L17             2 SEA ABB=ON  PLU=ON  L7/RCT(L)L8/PRO
                D SCAN
L18             4 SEA ABB=ON  PLU=ON  L8/RCT(L)L6/PRO
                D SCAN
L19             7 SEA ABB=ON  PLU=ON  (L15 OR L16 OR L17 OR L18)
                SAV L19 CHA440CRCT/A

     FILE 'STNGUIDE' ENTERED AT 15:44:09 ON 03 JAN 2008
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     FILE 'HCAPLUS' ENTERED AT 15:46:30 ON 03 JAN 2008
                D L1 AU
                E STUERMER R/AU
L20           74 SEA ABB=ON  PLU=ON  STUERMER R?/AU
                D SCAN L1
L21               QUE ABB=ON  PLU=ON  CHIRAL? OR ENANTIOMER? OR RESOLUTIO
                  N?
L22           35 SEA ABB=ON  PLU=ON  L20 AND L21
L23               QUE ABB=ON  PLU=ON  PY<2005 OR PRY<2005 OR AY<2005 OR
                  MY<2005 OR REVIEW/DT
L24           31 SEA ABB=ON  PLU=ON  L22 AND L23
                SAV TEMP L24 CHA440HCPIN/A

     FILE 'CASREACT' ENTERED AT 15:51:41 ON 03 JAN 2008
L25           32 SEA ABB=ON  PLU=ON  STUERMER R?/AU
L26           17 SEA ABB=ON  PLU=ON  L25 AND L21
L27           16 SEA ABB=ON  PLU=ON  L26 AND L23
                SAV TEMP L27 CHA440CRCTIN/A

     FILE 'HCAPLUS' ENTERED AT 15:52:48 ON 03 JAN 2008
                D SCAN L1
L28           27 SEA ABB=ON  PLU=ON  L5
L29           46 SEA ABB=ON  PLU=ON  L6
L30            9 SEA ABB=ON  PLU=ON  L28 AND L29
                D SCAN
L31            7 SEA ABB=ON  PLU=ON  L7
L32            5 SEA ABB=ON  PLU=ON  L28 AND L31
L33            9 SEA ABB=ON  PLU=ON  L8
L34            1 SEA ABB=ON  PLU=ON  L9
L35        11297 SEA ABB=ON  PLU=ON  L11
L36        34982 SEA ABB=ON  PLU=ON  L14
L37            2 SEA ABB=ON  PLU=ON  L31 AND ((L33 OR L34 OR L35 OR
                  L36))
                D SCAN
L38            5 SEA ABB=ON  PLU=ON  ((L33 OR L34)) AND L29
L39        19367 SEA ABB=ON  PLU=ON  L12
L40            1 SEA ABB=ON  PLU=ON  L38 AND L39
L41            8 SEA ABB=ON  PLU=ON  (L33 OR L34 OR L29) AND L39
                D SCAN
L42           10 SEA ABB=ON  PLU=ON  L30 OR L32 OR L37 OR L38 OR L40
L43           15 SEA ABB=ON  PLU=ON  L42 OR L41
L44           15 SEA ABB=ON  PLU=ON  L43 AND L23
                D SCAN
                SAV TEMP L44 CHA440HCP/A

     FILE 'STNGUIDE' ENTERED AT 16:02:51 ON 03 JAN 2008
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INVENTOR SEARCH

```
=> d his l27

     (FILE 'CASREACT' ENTERED AT 15:51:41 ON 03 JAN 2008)
L27          16 S L26 AND L23

=> d que l27
L21             QUE  ABB=ON  PLU=ON  CHIRAL? OR ENANTIOMER? OR RESOLUTI
                ON?
L23             QUE  ABB=ON  PLU=ON  PY<2005 OR PRY<2005 OR AY<2005 OR
                MY<2005 OR REVIEW/DT
L25          32 SEA FILE=CASREACT ABB=ON  PLU=ON  STUERMER R?/AU
L26          17 SEA FILE=CASREACT ABB=ON  PLU=ON  L25 AND L21
L27          16 SEA FILE=CASREACT ABB=ON  PLU=ON  L26 AND L23


=> d his l24

     (FILE 'HCAPLUS' ENTERED AT 15:46:30 ON 03 JAN 2008)
L24          31 S L22 AND L23

=> d que l24
L20          74 SEA FILE=HCAPLUS ABB=ON  PLU=ON  STUERMER R?/AU
L21             QUE  ABB=ON  PLU=ON  CHIRAL? OR ENANTIOMER? OR RESOLUTI
                ON?
L22          35 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20 AND L21
L23             QUE  ABB=ON  PLU=ON  PY<2005 OR PRY<2005 OR AY<2005 OR
                MY<2005 OR REVIEW/DT
L24          31 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L22 AND L23


=> dup rem l27 l24
FILE 'CASREACT' ENTERED AT 16:04:00 ON 03 JAN 2008
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'HCAPLUS' ENTERED AT 16:04:00 ON 03 JAN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)
PROCESSING COMPLETED FOR L27
PROCESSING COMPLETED FOR L24
L45          30 DUP REM L27 L24 (17 DUPLICATES REMOVED)
                ANSWERS '1-16' FROM FILE CASREACT
                ANSWERS '17-30' FROM FILE HCAPLUS
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INVENTOR SEARCH RESULTS

=> d 145 1-30 ibib ed

L45 ANSWER 1 OF 30 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 144:190717 CASREACT Full-text
TITLE: Lipase catalyzed enantioselective hydrolysis of oxetan-2-ones
INVENTOR(S): Habicher, Tilo; **Stuermer, Rainer**
PATENT ASSIGNEE(S): Basf Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 11 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006015727	A2	20060216	WO 2005-EP8190	20050728
WO 2006015727	A3	20060713		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
DE 102004037700	A1	20060316	DE 2004-102004037700 20040802	
DE 102004038589	A1	20060316	DE 2004-102004038589 20040806	
CN 1993472	A	20070704	CN 2005-80026005	20050728
EP 1805314	A2	20070711	EP 2005-769677	20050728
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				

PRIORITY APPLN. INFO.: DE 2004-102004037700 20040802
DE 2004-102004038589 20040806
WO 2005-EP8190 20050728
OTHER SOURCE(S): MARPAT 144:190717

L45 ANSWER 2 OF 30 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 143:192413 CASREACT Full-text
TITLE: A chemoenzymic synthesis of **enantiomerically** pure aminoalcohols
INVENTOR(S): **Stuermer, Rainer**
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 14 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2005073215 A1 20050811 WO 2005-EP420 20050118
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
DE 102004004719 A1 20050818 DE 2004-102004004719 20040129
EP 1713788 A1 20061025 EP 2005-700995 20050118
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS
CN 1914190 A 20070214 CN 2005-80003670 20050118
JP 2007519655 T 20070719 JP 2006-550005 20050118
US 2007128704 A1 20070607 US 2006-587440 20060726
PRIORITY APPLN. INFO.: DE 2004-102004004719 20040129
WO 2005-EP420 20050118
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 3 OF 30 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 142:392275 CASREACT Full-text
TITLE: enzymic and nonenzymic methods for the preparation of 3-methylamino-1-(thien-2-yl)propan-1-ol.
INVENTOR(S): **Stuermer, Rainer**; Kesseler, Maria; Hauer, Bernhard; Friedrich, Thomas; Breuer, Michael
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005033094	A2	20050414	WO 2004-EP10939	20040930
WO 2005033094	A3	20051124		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
DE 10345772 A1 20050421 DE 2003-10345772 20031001
EP 1670779 A2 20060621 EP 2004-765718 20040930
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR

CN 1860110	A	20061108	CN 2004-80028108	20040930
JP 2007533628	T	20071122	JP 2006-530058	20040930
US 2007083055	A1	20070412	US 2006-573130	20060517
PRIORITY APPLN. INFO.:			DE 2003-10345772	20031001
			WO 2004-EP10939	20040930

L45 ANSWER 4 OF 30 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 140:181317 CASREACT Full-text
TITLE: Preparation of **enantiomerically** pure (S)-3-methylamino-1-(thien-2-yl)propan-1-ol from racemic 3-hydroxy-3-(thien-2-yl)propionitrile via kinetic **resolution** with an acylating agent and a lipase followed by treatment with methylamine and hydrogen in the presence of a catalyst.
INVENTOR(S): **Stuermer, Rainer**
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004013123	A1	20040212	WO 2003-EP8492	20030731
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10235206	A1	20040219	DE 2002-10235206	20020801
CA 2493451	A1	20040212	CA 2003-2493451	20030731
AU 2003251677	A1	20040223	AU 2003-251677	20030731
EP 1527065	A1	20050504	EP 2003-766383	20030731
EP 1527065	B1	20061122		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1671687	A	20050921	CN 2003-818510	20030731
JP 2006507234	T	20060302	JP 2004-525403	20030731
AT 346061	T	20061215	AT 2003-766383	20030731
ES 2278203	T3	20070801	ES 2003-3766383	20030731
US 2005245749	A1	20051103	US 2005-522888	20050624
PRIORITY APPLN. INFO.:			DE 2002-10235206	20020801
			WO 2003-EP8492	20030731

L45 ANSWER 5 OF 30 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 141:23424 CASREACT Full-text
TITLE: Procedure for the production of N-(2-pyridyl)-1-amino-2-propanol from 2-aminopyridine and propylene oxide
INVENTOR(S): **Stuermer, Rainer**; Baldenius, Kai-uwe; Stratmann, Christian
PATENT ASSIGNEE(S): BASF Ag, Germany
SOURCE: Ger. Offen., 6 pp.

CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10254292	A1	20040603	DE 2002-10254292	20021120

PRIORITY APPLN. INFO.: DE 2002-10254292 20021120

L45 ANSWER 6 OF 30 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 6
ACCESSION NUMBER: 132:251248 CASREACT Full-text
TITLE: Process for asymmetric hydrogenation of keto esters with ruthenium catalysts having **chiral** bidentate bridged bis(phospholane) derivatives as ligands
INVENTOR(S): **Stuermer, Rainer**; Klatt, Martin Jochen; Boermer, Armin; Holz, Jens; Voss, Gudrun
PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: Ger. Offen., 12 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19845517	A1	20000406	DE 1998-19845517	19981002
EP 992481	A1	20000412	EP 1999-118428	19990917
EP 992481	B1	20030521		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
AT 240932	T	20030615	AT 1999-118428	19990917
ES 2200449	T3	20040301	ES 1999-118428	19990917
CA 2284162	A1	20000402	CA 1999-2284162	19990928
US 6359165	B1	20020319	US 1999-407283	19990929
JP 2000119217	A	20000425	JP 1999-278821	19990930

PRIORITY APPLN. INFO.: DE 1998-19845517 19981002
OTHER SOURCE(S): MARPAT 132:251248

L45 ANSWER 7 OF 30 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 7
ACCESSION NUMBER: 132:12408 CASREACT Full-text
TITLE: Preparation of optically active phospholanes, their metal complexes, and their use in asymmetric synthesis
INVENTOR(S): **Stuermer, Rainer**; Boerner, Armin; Holz, Jens; Voss, Gudrun
PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: Ger. Offen., 10 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19824121	A1	19991202	DE 1998-19824121	19980529
CA 2333888	A1	19991209	CA 1999-2333888	19990528
WO 9962917	A1	19991209	WO 1999-EP3702	19990528
W: CA, CN, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU,				

MC, NL, PT, SE

EP 1082328	A1	20010314	EP 1999-926460	19990528
EP 1082328	B1	20021120		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE, PT, IE				
JP 2002517403	T	20020618	JP 2000-552128	19990528
AT 228139	T	20021215	AT 1999-926460	19990528
ES 2188176	T3	20030616	ES 1999-926460	19990528
US 6632953	B1	20031014	US 2000-700521	20001115
PRIORITY APPLN. INFO.:			DE 1998-19824121	19980529
			WO 1999-EP3702	19990528

OTHER SOURCE(S): MARPAT 132:12408

L45 ANSWER 8 OF 30 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 8

ACCESSION NUMBER: 130:237655 CASREACT Full-text

TITLE: Asymmetric Thermal Transformation, a New Way to Enantiopure Biphenyl-Bridged Titanocene and Zirconocene Complexes: Efficient Catalysts for Asymmetric Imine Hydrogenation

AUTHOR(S): Ringwald, Markus; **Stuermer, Rainer**; Brintzinger, Hans H.

CORPORATE SOURCE: Fakultaet fuer Chemie, Universitaet Konstanz, Konstanz, D-78457, Germany

SOURCE: Journal of the American Chemical Society (**1999**), 121(7), 1524-1527
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 9 OF 30 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 9

ACCESSION NUMBER: 130:14028 CASREACT Full-text

TITLE: Synthesis of a New Class of Functionalized **Chiral** Bisphospholane Ligands and the Application in Enantioselective Hydrogenations

AUTHOR(S): Holz, Jens; Quirmbach, Michael; Schmidt, Ute; Heller, Detlef; **Stuermer, Rainer**; Boerner, Armin

CORPORATE SOURCE: Institut fuer Organische Katalyseforschung an der Universitaet Rostock e.V., Rostock, D-18055, Germany

SOURCE: Journal of Organic Chemistry (**1998**), 63(22), 8031-8034
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 10 OF 30 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 10

ACCESSION NUMBER: 128:89013 CASREACT Full-text

TITLE: **Chiral** organometalloheterocycles: synthesis and activity as enantioselective hydrogenation catalysts

INVENTOR(S): **Stuermer, Rainer**; Ritter, Kurt

PATENT ASSIGNEE(S): BASF A.-G., Germany

SOURCE: Ger. Offen., 10 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19622271 A1		**19971204**	DE 1996-19622271	**19960603**

OTHER SOURCE(S): MARPAT 128:89013

L45 ANSWER 11 OF 30 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 11
ACCESSION NUMBER: 126:293382 CASREACT Full-text
TITLE: Preparation of polyfunctional phosphines using zinc organometallics
AUTHOR(S): Langer, Falk; Puentener, Kurt; **Stuermer, Rainer**; Knochel, Paul
CORPORATE SOURCE: Fachbereich Chemie der Philipps-Universitat Marburg, Marburg, D-35032, Germany
SOURCE: Tetrahedron: Asymmetry (**1997**), 8(5), 715-738
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 12 OF 30 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 12
ACCESSION NUMBER: 126:60177 CASREACT Full-text
TITLE: Preparation of optically active phosphine and their metal complexes and their use in asymmetric synthesis
INVENTOR(S): **Stuermer, Rainer**; Laupichler, Lothar; Knochel, Paul; Falk, Langer
PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: Ger. Offen., 6 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19516968	A1	19961114	DE 1995-19516968	19950512
US 5723642	A	19980303	US 1996-643586	19960506
EP 743316	A2	19961120	EP 1996-107261	19960508
EP 743316	A3	19980429		
EP 743316	B1	20021106		
R: CH, DE, FR, GB, LI				
CA 2176304	A1	19961113	CA 1996-2176304	19960510
CA 2176304	C	20070109		
PRIORITY APPLN. INFO.:			DE 1995-19516968	19950512

OTHER SOURCE(S): MARPAT 126:60177

L45 ANSWER 13 OF 30 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 13
ACCESSION NUMBER: 126:74998 CASREACT Full-text
TITLE: Optically active titanium complexes containing linked amido cyclopentadienyl ligands. Their use as asymmetric hydrogenation catalysts
AUTHOR(S): Okuda, Jun; Verch, Sabine; Spaniol, Thomas P.; **Stuermer, Rainer**
CORPORATE SOURCE: Institut Anorganische Chemie Analytische Chemie, Universitaet Mainz, Mainz, D-55099,

Germany
SOURCE: Chemische Berichte (**1996**), 129(12), 1429-1431
CODEN: CHBEAM; ISSN: 0009-2940
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English

L45 ANSWER 14 OF 30 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 14
ACCESSION NUMBER: 114:206505 CASREACT Full-text
TITLE: Enantioselective allylboration of aldehydes with (4R,5R)-2-[(S)-1-chloro-2-propenyl]-4,5-dicyclohexyl-1,3,2-dioxaborolane
AUTHOR(S): **Stuermer, Rainer**; Hoffmann, Reinhard W.
CORPORATE SOURCE: Fachbereich Chem., Philipps-Univ. Marburg, Marburg, D-3550, Germany
SOURCE: Synlett (**1990**), (12), 759-61
CODEN: SYNLES; ISSN: 0936-5214
DOCUMENT TYPE: Journal
LANGUAGE: English

L45 ANSWER 15 OF 30 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 15
ACCESSION NUMBER: 112:118887 CASREACT Full-text
TITLE: A new pathway to highly **enantiomer** enriched (Z)-1-methyl-2-butenylboronic acid esters
AUTHOR(S): **Stuermer, Rainer**
CORPORATE SOURCE: Fachbereich Chem., Univ. Marburg, Marburg, D-3550, Germany
SOURCE: Angewandte Chemie (**1990**), 102(1), 62
CODEN: ANCEAD; ISSN: 0044-8249
DOCUMENT TYPE: Journal
LANGUAGE: German

L45 ANSWER 16 OF 30 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 16
ACCESSION NUMBER: 111:153467 CASREACT Full-text
TITLE: Stereoselective synthesis of alcohols. XXXI. Stereoselective carbon-carbon bond formation using **chiral** Z-pentenylboronates
AUTHOR(S): Hoffmann, Reinhard W.; Ditrich, Klaus; Koester, Gerhard; **Stuermer, Rainer**
CORPORATE SOURCE: Fachbereich Chem., Philipps-Univ., Marburg, D-3550, Fed. Rep. Ger.
SOURCE: Chemische Berichte (**1989**), 122(9), 1783-9
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: English

L45 ANSWER 17 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:393385 HCAPLUS Full-text
DOCUMENT NUMBER: 147:72240
TITLE: Asymmetric bioreduction of activated C:C bonds using enoate reductases from the old yellow enzyme family
AUTHOR(S): **Stuermer, Rainer**; Hauer, Bernhard; Hall, Melanie; Faber, Kurt
CORPORATE SOURCE: BASF AG, GVF/E-B9, Ludwigshafen, D-67056, Germany
SOURCE: Current Opinion in Chemical Biology (2007), 11(2), 203-213
CODEN: COCBF4; ISSN: 1367-5931
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal; **General Review**
LANGUAGE: English
ED Entered STN: 09 Apr 2007
REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 18 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:446669 HCAPLUS Full-text
DOCUMENT NUMBER: 145:27376
TITLE: Enzymes as catalysts. Chemistry and biology hand in hand
AUTHOR(S): **Stuermer, Rainer**; Breuer, Michael
CORPORATE SOURCE: BASF Aktiengesellschaft, Ludwigshafen, 67056, Germany
SOURCE: Chemie in Unserer Zeit (2006), 40(2), 104-111
CODEN: CUNZAW; ISSN: 0009-2851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal; **General Review**
LANGUAGE: German
ED Entered STN: 12 May 2006
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 19 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1220820 HCAPLUS Full-text
DOCUMENT NUMBER: 143:458684
TITLE: Enzymic production of **chiral** alcohols using Azoarcus strain EbN1 S)-1-phenylethanol dehydrogenase
INVENTOR(S): **Stuermer, Rainer**; Kesseler, Maria; Hauer, Bernhard; Friedrich, Thomas; Breuer, Michael; Schroeder, Hartwig
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005108590	A2	20051117	WO 2005-EP4872	2005 0504
			<--	
WO 2005108590	A3	20060406		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 102004022686	A1	20051124	DE 2004-102004022686	2004 0505
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EP 1745133	A2	20070124	EP 2005-745555	

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0504
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R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR

CN 1950513 A 20070418 CN 2005-80014367
2005
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JP 2007535956 T 20071213 JP 2007-512023
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PRIORITY APPLN. INFO.: DE 2004-102004022686A
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WO 2005-EP4872 W
2005
0504

OTHER SOURCE(S): MARPAT 143:458684
ED Entered STN: 18 Nov 2005

L45 ANSWER 20 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:158288 HCAPLUS Full-text
DOCUMENT NUMBER: 140:302346
TITLE: Industrial methods for the production of optically active intermediates
AUTHOR(S): Breuer, Michael; Ditrich, Klaus; Habicher, Tilo; Hauer, Bernhard; Kesseler, Maria; **Stuermer, Rainer**; Zelinski, Thomas
CORPORATE SOURCE: Forschung Feinchemikalien & Biokatalyse, BASF Aktiengesellschaft, Ludwigshafen, 67056, Germany
SOURCE: Angewandte Chemie, International Edition (**2004**), 43(7), 788-824
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal; **General Review**
LANGUAGE: English
ED Entered STN: 27 Feb 2004
REFERENCE COUNT: 393 THERE ARE 393 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 21 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:331990 HCAPLUS Full-text
DOCUMENT NUMBER: 138:350486
TITLE: Oxyanion hole variants of lipases with increased specific activity for use in catalysis of stereospecific esterification and hydrolysis
INVENTOR(S): Matuschek, Markus; **Stuermer, Rainer**; Hauer, Bernhard; Klebe, Gerhard; Bocola, Marco
PATENT ASSIGNEE(S): BASF AG, Germany
SOURCE: Ger. Offen., 16 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DE 10151292 A1 20030430 DE 2001-10151292
2001
1022
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WO 2003035878 A2 20030501 WO 2002-EP11620
2002
1017
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WO 2003035878 A3 20040311
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
AU 2002346934 A1 20030506 AU 2002-346934
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EP 1440155 A2 20040728 EP 2002-782936
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
JP 2005506088 T 20050303 JP 2003-538378
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US 2005255571 A1 20051117 US 2004-493210
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US 7314739 B2 20080101
PRIORITY APPLN. INFO.: DE 2001-10151292 A
2001
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DE 2002-10205444 A
2002
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WO 2002-EP11620 W
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ED Entered STN: 01 May 2003

L45 ANSWER 22 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:172063 HCAPLUS Full-text
DOCUMENT NUMBER: 136:228758
TITLE: Butinol I esterase from Pseudomonas glumae for use in enantioselective hydrolysis and cloning and expression of the gene for the enzyme
INVENTOR(S): Hauer, Bernhard; Friedrich, Thomas; Nuebling, Christoph; **Stuermer, Rainer**
PATENT ASSIGNEE(S): Basf Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002018560	A2	20020307	WO 2001-EP10040	20010830
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WO 2002018560	A3	20021031		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10042892	A1	20020314	DE 2000-10042892	20000831
			<--	
DE 10131544	A1	20030116	DE 2001-10131544	20010629
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CA 2419275	A1	20020307	CA 2001-2419275	20010830
			<--	
AU 200184047	A	20020313	AU 2001-84047	20010830
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EP 1313860	A2	20030528	EP 2001-962989	20010830
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004507268	T	20040311	JP 2002-524063	20010830
			<--	
EE 200300086	A	20041215	EE 2003-86	20010830
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AU 2001284047	B2	20070329	AU 2001-284047	20010830
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MX 2003PA01333	A	20030606	MX 2003-PA1333	20030213
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US 2005181472	A1	20050818	US 2003-362530	20030225
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PRIORITY APPLN. INFO.:			DE 2000-10042892 A	20000831

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DE 2001-10131544 A
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WO 2001-EP10040 W
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OTHER SOURCE(S): MARPAT 136:228758
ED Entered STN: 08 Mar 2002

L45 ANSWER 23 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:463997 HCAPLUS Full-text
DOCUMENT NUMBER: 137:48866
TITLE: Racemization of optically active amines
INVENTOR(S): Funke, Frank; Liang, Shelue; Kramer, Andreas; **Stuermer, Rainer**; Hoehn, Arthur
PATENT ASSIGNEE(S): Basf Aktiengesellschaft, Germany
SOURCE: Eur. Pat. Appl., 14 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1215197	A2	20020619	EP 2001-128602	2001 1130
			<--	
EP 1215197	A3	20031029		
EP 1215197	B1	20050223		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
DE 10062729	A1	20020620	DE 2000-10062729	2000 1215
			<--	
AT 289582	T	20050315	AT 2001-128602	2001 1130
			<--	
ES 2237523	T3	20050801	ES 2001-1128602	2001 1130
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US 2002120166	A1	20020829	US 2001-12344	2001 1212
			<--	
US 6548704	B2	20030415		
CN 1363549	A	20020814	CN 2001-142892	2001 1214
			<--	
JP 2002226437	A	20020814	JP 2001-383504	2001 1217
			<--	
US 6576795	B1	20030610	US 2002-261123	2002 1001
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PRIORITY APPLN. INFO.: DE 2000-10062729 A

2000
1215
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US 2001-12344 A3
2001
1212
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OTHER SOURCE(S): MARPAT 137:48866
ED Entered STN: 21 Jun 2002

L45 ANSWER 24 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:780338 HCAPLUS Full-text
DOCUMENT NUMBER: 135:328762
TITLE: Procedure for covalent immobilization of biologically active materials on polyurethane foams for use in **chiral** synthesis
INVENTOR(S): Falke, Peter; Hendreich, Regina; **Stuermer, Rainer**; Friedrich, Thomas
PATENT ASSIGNEE(S): Basf A.-G., Germany
SOURCE: Ger. Offen., 10 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10019380	A1	20011025	DE 2000-10019380	2000 0419 <--
EP 1149849	A1	20011031	EP 2001-107566	2001 0327 <--
EP 1149849	B1	20030528		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
AT 241656	T	20030615	AT 2001-107566	2001 0327 <--

PRIORITY APPLN. INFO.: DE 2000-10019380 A 2000 0419 <--

ED Entered STN: 26 Oct 2001

L45 ANSWER 25 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:780337 HCAPLUS Full-text
DOCUMENT NUMBER: 135:315323
TITLE: Immobilization of biologically active materials on polymer foams for use in **chiral** synthesis
INVENTOR(S): Falke, Peter; Hendreich, Regina; **Stuermer, Rainer**; Friedrich, Thomas
PATENT ASSIGNEE(S): Basf A.-G., Germany
SOURCE: Ger. Offen., 8 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

DE 10019377	A1	20011025	DE 2000-10019377 <--	2000 0419
PRIORITY APPLN. INFO.:			DE 2000-10019377 <--	2000 0419

ED Entered STN: 26 Oct 2001

L45 ANSWER 26 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:36756 HCAPLUS Full-text
DOCUMENT NUMBER: 132:207902
TITLE: Optically Active Transition-Metal Complexes. 10.1 Bifunctional Arene-Chromium-Tricarbonyl Complexes Derived from (R)-Phenylethanamine: Easily Accessible Planar-**Chiral** Diphosphines and Their Application in Enantioselective Hydrogenation, Hydroamination, and Allylic Sulfonation
AUTHOR(S): Vasen, Daniela; Salzer, A.; Gerhards, Frank; Gais, Hans-Joachim; **Stuermer, Rainer**; Bieler, Nikolaus H.; Togni, Antonio
CORPORATE SOURCE: Institut fuer Anorganische Chemie, RWTH Aachen, Aachen, D 52056, Germany
SOURCE: Organometallics (**2000**), 19(4), 539-546
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 18 Jan 2000
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 27 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:35084 HCAPLUS Full-text
DOCUMENT NUMBER: 130:66802
TITLE: **Resolution** of racemic amino acid esters by enzyme-catalyzed acylation
INVENTOR(S): **Stuermer, Rainer**; Ditrich, Klaus; Siegel, Wolfgang
PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: Ger. Offen., 6 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19727517	A1	19990107	DE 1997-19727517 <--	1997 0630
EP 890649	A1	19990113	EP 1998-109999 <--	1998 0602
EP 890649	B1	20040303		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

AT 260984	T	20040315	AT 1998-109999	1998 0602 <--
ES 2217452	T3	20041101	ES 1998-109999	1998 0602 <--
IN 1998MA01407	A	20050304	IN 1998-MA1407	1998 0624 <--
CN 1203949	A	19990106	CN 1998-115528	1998 0629 <--
CN 1102661	B	20030305		
JP 11069992	A	19990316	JP 1998-184055	1998 0630 <--
PRIORITY APPLN. INFO.:			DE 1997-19727517 A	1997 0630 <--

OTHER SOURCE(S): MARPAT 130:66802
ED Entered STN: 19 Jan 1999

L45 ANSWER 28 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:459656 HCAPLUS Full-text
DOCUMENT NUMBER: 131:286585
TITLE: Asymmetric Thermal Transformation, a New Way to Enantiopure Biphenyl-Bridged Titanocene and Zirconocene Complexes: Efficient Catalysts for Asymmetric Imine Hydrogenation. [Erratum to document cited in CA130:237655]
AUTHOR(S): Ringwald, Markus; **Stuermer, Rainer**; Brintzinger, Hans H.
CORPORATE SOURCE: Fakultaet fuer Chemie, Universitaet Konstanz, Konstanz, D-78457, Germany
SOURCE: Journal of the American Chemical Society (**1999**), 121(31), 7278
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 28 Jul 1999

L45 ANSWER 29 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:148796 HCAPLUS Full-text
DOCUMENT NUMBER: 126:157639
TITLE: Transformation of achiral meso-form or racemates of ansa-metallocene complexes or their mixture to the pure **enantiomeric** form
INVENTOR(S): Fischer, David; Langhauser, Franz; **Stuermer, Rainer**; Kerth, Juergen; Schweier, Guenther; Brintzinger, Hans-Herbert; Schmidt, Katrin
PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: Ger. Offen., 12 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19525184	A1	19970116	DE 1995-19525184	1995 0711
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WO 9703081	A1	19970130	WO 1996-EP2869	1996 0701
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W: CN, JP, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 837866	A1	19980429	EP 1996-924832	1996 0701
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EP 837866	B1	20011114		
R: AT, BE, DE, ES, FR, GB, IT, NL, FI				
CN 1190399	A	19980812	CN 1996-195406	1996 0701
			<--	
CN 1065867	B	20010516		
JP 11508597	T	19990727	JP 1997-505468	1996 0701
			<--	
AT 208786	T	20011115	AT 1996-924832	1996 0701
			<--	
US 5840950	A	19981124	US 1998-981638	1998 0108
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PRIORITY APPLN. INFO.:			DE 1995-19525184 A	1995 0711
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			WO 1996-EP2869 W	1996 0701
			<--	

OTHER SOURCE(S): MARPAT 126:157639
ED Entered STN: 07 Mar 1997

L45 ANSWER 30 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:263727 HCAPLUS Full-text
DOCUMENT NUMBER: 122:213812
TITLE: Stereoselective synthesis of alcohols. XLVII. Application of **chiral** Z-pentenylboronates to the synthesis of erythronolide building blocks
AUTHOR(S): Hoffmann, Reinhard W.; **Stuermer, Rainer**
CORPORATE SOURCE: Fachbereich Chemie, Philipps-Universitaet Marburg, Marburg, D-35032, Germany
SOURCE: Chemische Berichte (**1994**), 127(12), 2511-18
CODEN: CHBEAM; ISSN: 0009-2940
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 24 Dec 1994

TEXT SEARCH

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     (FILE 'CASREACT' ENTERED AT 15:31:03 ON 03 JAN 2008)
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L7           1 SEA FILE=REGISTRY ABB=ON  PLU=ON  260354-12-9/RN
L8           1 SEA FILE=REGISTRY ABB=ON  PLU=ON  164071-56-1/RN
L15          6 SEA FILE=CASREACT ABB=ON  PLU=ON  L5/RCT(L)L6/PRO
L16          4 SEA FILE=CASREACT ABB=ON  PLU=ON  L5/RCT(L)L7/PRO
L17          2 SEA FILE=CASREACT ABB=ON  PLU=ON  L7/RCT(L)L8/PRO
L18          4 SEA FILE=CASREACT ABB=ON  PLU=ON  L8/RCT(L)L6/PRO
L19          7 SEA FILE=CASREACT ABB=ON  PLU=ON  (L15 OR L16 OR L17
               OR L18)


=> d his l44

     (FILE 'HCAPLUS' ENTERED AT 15:52:48 ON 03 JAN 2008)
L44         15 S L43 AND L23

=> d que stat l44
L5           1 SEA FILE=REGISTRY ABB=ON  PLU=ON  40570-64-7/RN
L6           1 SEA FILE=REGISTRY ABB=ON  PLU=ON  116539-55-0/RN
L7           1 SEA FILE=REGISTRY ABB=ON  PLU=ON  260354-12-9/RN
L8           1 SEA FILE=REGISTRY ABB=ON  PLU=ON  164071-56-1/RN
L9           1 SEA FILE=REGISTRY ABB=ON  PLU=ON  861995-99-5/RN
L11          1 SEA FILE=REGISTRY ABB=ON  PLU=ON  108-30-5/RN
L12          1 SEA FILE=REGISTRY ABB=ON  PLU=ON  METHANAMINE/CN
L14          1 SEA FILE=REGISTRY ABB=ON  PLU=ON  9001-62-1/RN
L23            QUE  ABB=ON  PLU=ON  PY<2005 OR PRY<2005 OR AY<2005 OR
               MY<2005 OR REVIEW/DT
L28         27 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L5
L29         46 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L6
L30          9 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L28 AND L29
L31          7 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L7
L32          5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L28 AND L31
L33          9 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L8
L34          1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L9
L35      11297 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L11
L36      34982 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L14
L37          2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L31 AND ((L33 OR L34
               OR L35 OR L36))
L38          5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ((L33 OR L34)) AND
               L29
L39      19367 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L12
L40          1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L38 AND L39
L41          8 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L33 OR L34 OR L29)
               AND L39
L42         10 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L30 OR L32 OR L37 OR
               L38 OR L40
L43         15 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L42 OR L41
L44         15 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L43 AND L23


=> dup rem l19 l44
PROCESSING COMPLETED FOR L19
PROCESSING COMPLETED FOR L44
L46         15 DUP REM L19 L44 (7 DUPLICATES REMOVED)
               ANSWERS '1-7' FROM FILE CASREACT
               ANSWERS '8-15' FROM FILE HCAPLUS
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TEXT SEARCH RESULTS

=> d l46 1-7 ibib ab fhit ind

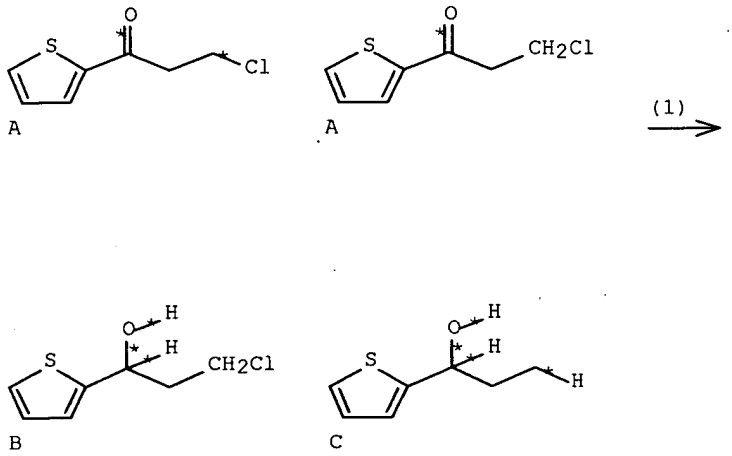
L46 ANSWER 1 OF 15 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 143:192413 CASREACT Full-text
TITLE: A chemoenzymic synthesis of enantiomerically pure aminoalcohols
INVENTOR(S): Stuermer, Rainer
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 14 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005073215	A1	20050811	WO 2005-EP420	20050118
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 102004004719	A1	20050818	DE 2004-102004004719	20040129
EP 1713788	A1	20061025	EP 2005-700995	20050118
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
CN 1914190	A	20070214	CN 2005-80003670	20050118
JP 2007519655	T	20070719	JP 2006-550005	20050118
US 2007128704	A1	20070607	US 2006-587440	20060726

PRIORITY APPLN. INFO.: DE 2004-102004004719 20040129
WO 2005-EP420 20050118

AB A process is provided for the chemoenzymic synthesis of (1S)-3-methylamino-1-(2-thienyl)-propan-1-ol from 3-chloro-1-(2-thienyl)-1-propanone using a three step procedure. First, 3-chloro-1-(2-thienyl)-1-propanone is chemical reduced to 3-chloro-1-(2-thienyl)-1-propanol using sodium borohydride. This product is then stereoselectively acylated succinic anhydride in a kinetic resolution catalyzed by an immobilized lipase. The unreacted 3S-chloro-1-(2-thienyl)-1-propanol is separated from the R conjugate base and then aminated with methylamine to form (1S)-3-methylamino-1-(2-thienyl)-propan-1-ol.

RX(1) OF 6 2 **A** ===> **B** + C...



RX(1) RCT A **40570-64-7**

STAGE(1)
RGT D 16940-66-2 NaBH4, E 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH, 108-88-3 PhMe
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 2.5 hours, 0 deg C
SUBSTAGE(3) 40 minutes, 0 deg C

STAGE(2)
RGT F 64-19-7 AcOH
SOL 7732-18-5 Water
CON 0 deg C

PRO B **260354-12-9**, C 23229-69-8

IC ICM C07D333-14
ICS C07D333-20
CC 16-5 (Fermentation and Bioindustrial Chemistry)
Section cross-reference(s): 27
ST chiral aminoalc synthesis chemoenzymic
IT Amination
Crystallization
Reduction
(chemoenzymic synthesis of enantiomerically pure aminoalcs.)
IT Hydrocarbons, processes
RL: BCP (Biochemical process); BIOL (Biological study); PROC (Process)
(chemoenzymic synthesis of enantiomerically pure aminoalcs.)
IT Alcohols, preparation
RL: IMF (Industrial manufacture); PRP (Properties); PUR (Purification or recovery); PREP (Preparation)
(chiral, amino; chemoenzymic synthesis of enantiomerically pure aminoalcs.)
IT Burkholderia
Pseudomonas
(claimed lipase source; chemoenzymic synthesis of enantiomerically pure aminoalcs.)
IT Acylation
(enzymic, Stereoselective; chemoenzymic synthesis of enantiomerically pure aminoalcs.)
IT Resolution (separation)
(enzymic, kinetic; chemoenzymic synthesis of enantiomerically pure aminoalcs.)
IT Enzymes, uses

RL: BCP (Biochemical process); CAT (Catalyst use); BIOL (Biological study); PROC (Process); USES (Uses)
(immobilized; chemoenzymic synthesis of enantiomerically pure aminoalcs.)

IT Acylation
(stereoselective, enzymic; chemoenzymic synthesis of enantiomerically pure aminoalcs.)

IT 9001-62-1, Lipase
RL: BCP (Biochemical process); CAT (Catalyst use); BIOL (Biological study); PROC (Process); USES (Uses)
(chemoenzymic synthesis of enantiomerically pure aminoalcs.)

IT 108-30-5, Succinic anhydride, reactions
RL: BCP (Biochemical process); RCT (Reactant); BIOL (Biological study); PROC (Process); RACT (Reactant or reagent)
(chemoenzymic synthesis of enantiomerically pure aminoalcs.)

IT 164071-56-1P
RL: BPN (Biosynthetic preparation); CPS (Chemical process); PEP (Physical, engineering or chemical process); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(chemoenzymic synthesis of enantiomerically pure aminoalcs.)

IT 23229-69-8P 861995-99-5P
RL: BYP (Byproduct); PREP (Preparation)
(chemoenzymic synthesis of enantiomerically pure aminoalcs.)

IT 96-49-1, Ethylene carbonate 108-32-7, Propylene carbonate 142-82-5, Heptane, processes
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PROC (Process)
(chemoenzymic synthesis of enantiomerically pure aminoalcs.)

IT 260354-12-9P, 3-Chloro-1-(2-thienyl)-propan-1-ol
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(chemoenzymic synthesis of enantiomerically pure aminoalcs.)

IT 74-89-5, Methylamine, reactions 16940-66-2, Sodium borohydride 40570-64-7
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(chemoenzymic synthesis of enantiomerically pure aminoalcs.)

IT 116539-55-0P
RL: IMF (Industrial manufacture); PRP (Properties); PUR (Purification or recovery); PREP (Preparation)
(chemoenzymic synthesis of enantiomerically pure aminoalcs.)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 2 OF 15 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 142:392275 CASREACT Full-text

TITLE: enzymic and nonenzymic methods for the preparation of 3-methylamino-1-(thien-2-yl)propan-1-ol.

INVENTOR(S): Stuermer, Rainer; Kesseler, Maria; Hauer, Bernhard; Friedrich, Thomas; Breuer, Michael

PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

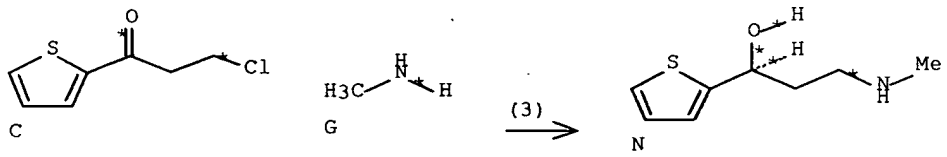
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2005033094 A2 20050414 WO 2004-EP10939 20040930
WO 2005033094 A3 20051124
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
DE 10345772 A1 20050421 DE 2003-10345772 20031001
EP 1670779 A2 20060621 EP 2004-765718 20040930
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
CN 1860110 A 20061108 CN 2004-80028108 20040930
JP 2007533628 T 20071122 JP 2006-530058 20040930
US 2007083055 A1 20070412 US 2006-573130 20060517
PRIORITY APPLN. INFO.: DE 2003-10345772 20031001
WO 2004-EP10939 20040930

AB The invention relates to enzymic and non-enzymic methods for the production of 3-methylamino-1-(thien-2-yl)propan-1-ol, o enzymes for carrying out said method, nucleic acid sequences coding for said enzymes, expression cassettes containing them, vectors and recombinant hosts. A process for preparation of 3-methylamino-1-(thien-2-yl)propan- 1-ol comprises reaction of thiophene with a β-halopropionyl halide or an acryloyl halide in the presence of a Lewis acid to obtain a 3-halo-1-(thien-2-yl)propan-1-one, reduction, and treatment with MeNH2. A hydrogen halide is added during or after the first reaction step but before isolation of propanone product. (S)-3-methylamino-1-(thien-2-yl)propan-1-ol is prepared via treatment of the propanone with a chiral reducing agent. Thus, thiophene in dichloroethane was treated with AlCl3 and then with 3-chloropropionyl chloride followed by stirring for 12 h and addition of gaseous HCl to give 96% 3-chloro-1-(thien-2-yl)propan-1-one. The latter in PhMe/MeOH at 0° was treated with 30% aqueous NaOH and then with NaBH4; after 40 min. aqueous MeNH2 was added followed by stirring for 6 h at 60° to give 3-methylamino-1-(thien-2-yl)propan-1-ol.

RX(3) OF 5 ...C + G ===> N



RX(3) RCT C **40570-64-7**, G 74-89-5

STAGE(1)
SOL 7732-18-5 Water
CON 6 hours, 60 deg C

STAGE(2)
CAT 9001-62-1 Lipase

PRO N **116539-55-0**

NTE biotransformation, described medium, stereoselective, dehydrogenase from Lactobacillus brevis used as catalyst in second stage

IC ICM C07D333-16

CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 16

ST methylaminothienylpropanol enzymic nonenzymic prepn; thienylpropanol methylamino enzymic nonenzymic prepn; thiophenemethanol methylaminoethyl prepn enzymic nonenzymic; thiophene chloropropionyl chloride Friedel Crafts reaction; thienylchloropropanone redn amination enzymic chem

IT Alcohols, preparation
RL: BPN (Biosynthetic preparation); IMF (Industrial manufacture); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(chiral; enzymic and nonenzymic methods for the preparation of methylaminothienylpropanol)

IT Asymmetric synthesis and induction
Friedel-Crafts reaction
Reduction
(enzymic and nonenzymic methods for the preparation of methylaminothienylpropanol)

IT Lewis acids
RL: CAT (Catalyst use); USES (Uses)
(enzymic and nonenzymic methods for the preparation of methylaminothienylpropanol)

IT Reduction
(enzymic; enzymic and nonenzymic methods for the preparation of methylaminothienylpropanol)

IT 116539-55-0P, (S)-3-Methylamino-1-(thien-2-yl)propan-1-ol
RL: BPN (Biosynthetic preparation); IMF (Industrial manufacture); BIOL (Biological study); PREP (Preparation)
(enzymic and nonenzymic methods for the preparation of methylaminothienylpropanol)

IT 7446-70-0, Aluminum chloride, uses 9028-12-0, e.c.1.1.1.2 9028-53-9, Glucose dehydrogenase 9031-72-5, e.c.1.1.1.1 9035-82-9, Dehydrogenase
RL: CAT (Catalyst use); USES (Uses)
(enzymic and nonenzymic methods for the preparation of methylaminothienylpropanol)

IT 116539-56-1P, 3-Methylamino-1-(thien-2-yl)propan-1-ol
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(enzymic and nonenzymic methods for the preparation of methylaminothienylpropanol)

IT 67-56-1, Methanol, uses 108-88-3, Toluene, uses 1300-21-6, Dichloroethane
RL: NUU (Other use, unclassified); USES (Uses)
(enzymic and nonenzymic methods for the preparation of methylaminothienylpropanol)

IT 74-89-5, Methylamine, reactions 110-02-1, Thiophene 625-36-5, 3-Chloropropionyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(enzymic and nonenzymic methods for the preparation of methylaminothienylpropanol)

IT 40570-64-7P, 3-Chloro-1-(thien-2-yl)propan-1-one
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enzymic and nonenzymic methods for the preparation of methylaminothienylpropanol)

IT 53-57-6, Nadph 58-68-4, Nadh 7647-01-0, Hydrogen chloride, reactions
RL: RGT (Reagent); RACT (Reactant or reagent)
(enzymic and nonenzymic methods for the preparation of methylaminothienylpropanol)

IT 849850-91-5 849850-93-7 849850-95-9 849850-96-0 849850-97-1 849850-98-2 849850-99-3

RL: PRP (Properties)
(unclaimed nucleotide sequence; enzymic and nonenzymic methods for the preparation of 3-methylamino-1-(thien-2-yl)propan-1-ol.)

IT 849850-90-4 849850-92-6 849850-94-8 850101-05-2
RL: PRP (Properties)
(unclaimed protein sequence; enzymic and nonenzymic methods for the preparation of 3-methylamino-1-(thien-2-yl)propan-1-ol.)

IT 849819-89-2
RL: PRP (Properties)
(unclaimed sequence; enzymic and nonenzymic methods for the preparation of 3-methylamino-1-(thien-2-yl)propan-1-ol.)

L46 ANSWER 3 OF 15 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 140:77017 CASREACT Full-text
TITLE: Process for preparation of an optically active isomer of heteroarylmonoalkylaminoalkanols, in particular (S)-1-(2-Thiophene)-3-methylamino-1-propanol, by resolution of their racemates with diprogulic acid diprogulic acid
INVENTOR(S): Roussiasse, Sonia; Frein, Stephane; Burgos, Alain; Bertrand, Blandine; Clementz, Myriam; Total, Avril
PATENT ASSIGNEE(S): PPG-Sipsy, Fr.
SOURCE: Fr. Demande, 16 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2841899	A1	20040109	FR 2002-8516	20020705
WO 2004005220	A2	20040115	WO 2003-FR2086	20030704
WO 2004005220	A3	20040415		

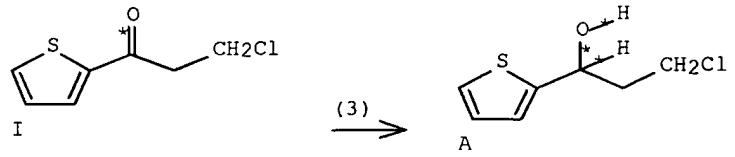
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2003263264	A1	20040123	AU 2003-263264	20030704
PRIORITY APPLN. INFO.:			FR 2002-8516	20020705
			WO 2003-FR2086	20030704

OTHER SOURCE(S): MARPAT 140:77017

AB The invention is directed to a process for preparation of an optically active isomer of I by resolution of its racemate with diprogulic acid or a salt of this acid [wherein Ar = heteroaryl; R1 = alkyl; R2, R3 = independently H, alkyl; X = (CH2)n; n = 0-4]. The advantage includes the preparation of desired optically active heteroarylmonoalkylaminoalkanols, in particular (S)-II, well-known intermediate in the synthesis of duloxetine. For example, (S)-II was prepared by resolution of racemic-II with diprogulic acid in 2-propanol, recrystn. from ethanol to give II•diprogulic acid in 91% yield and 95% d.e., followed by hydrolysis. Racemic-II was prepared by acylation of thiophene with propionyl chloride, reduction with NaBH4/EtOH, and alkylation with methylamine.

RX(3) OF 12 ...I ===> A...



RX(3)

STAGE(1)
RGT L 16940-66-2 NaBH4
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 15 minutes, room temperature
SUBSTAGE(2) room temperature -> -6 deg C

STAGE(2)
RCT I **40570-64-7**
CON 40 minutes, -2 deg C

STAGE(3)
SOL 75-09-2 CH2Cl2
CON 1 hour, -3 deg C

STAGE(4)
RGT M 12125-02-9 NH4Cl
SOL 7732-18-5 Water
CON SUBSTAGE(1) 40 minutes, -3 - 0 deg C
SUBSTAGE(2) 2 hours, room temperature

PRO A **260354-12-9**

IC ICM C07B055-00
ICS C07D333-20
CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 45
ST heteroarylmonoalkylaminoalkanol prepn resoln racemic diprogulic acid; thiophene methylaminopropanol prepn resoln racemic diprogulic acid
IT Resolution (separation)
(of racemic; process for preparation of optically active heteroarylmonoalkylaminoalkanols by resolution of its racemates with diprogulic acid diprogulic acid)
IT Alcohols, preparation
RL: IMF (Industrial manufacture); PREP (Preparation)
(secondary, chiral, chiral alc. product; process for preparation of optically active heteroarylmonoalkylaminoalkanols by resolution of its racemates with diprogulic acid diprogulic acid)
IT Alcohols, preparation
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(secondary, intermediate; process for preparation of optically active heteroarylmonoalkylaminoalkanols by resolution of its racemates with diprogulic acid diprogulic acid)
IT 625-36-5, 3-Chloropropionyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(Friedel-Crafts acylation by, of thiophene; process for preparation of optically active heteroarylmonoalkylaminoalkanols by resolution of its racemates with diprogulic acid diprogulic acid)
IT 110-02-1, Thiophene
RL: RCT (Reactant); RACT (Reactant or reagent)
(Friedel-Crafts acylation of, with chloropropionyl chloride;

process for preparation of optically active heteroarylmonoalkylaminoalkanols by resolution of its racemates with diprogulic acid diprogulic acid)

IT 116539-55-0P
RL: IMF (Industrial manufacture); PREP (Preparation)
(chiral thiophenylalc. product; process for preparation of optically active heteroarylmonoalkylaminoalkanols by resolution of its racemates with diprogulic acid diprogulic acid)

IT 569687-76-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(diastereomeric salt intermediate; process for preparation of optically active heteroarylmonoalkylaminoalkanols by resolution of its racemates with diprogulic acid diprogulic acid)

IT 40570-64-7P, 3-Chloro-1-(2-thiophene)propanone 116539-56-1P
260354-12-9P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; process for preparation of optically active heteroarylmonoalkylaminoalkanols by resolution of its racemates with diprogulic acid diprogulic acid)

IT 18467-77-1, Diprogulic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(resolving agent; process for preparation of optically active heteroarylmonoalkylaminoalkanols by resolution of its racemates with diprogulic acid diprogulic acid)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

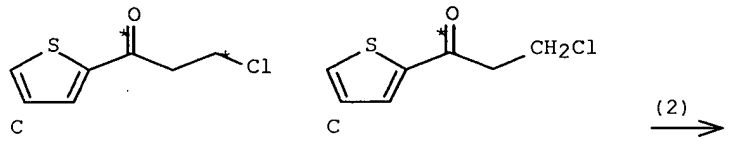
L46 ANSWER 4 OF 15 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 140:357198 CASREACT Full-text
TITLE: Procedure for the production of thienyl-substituted secondary aminoalcohols
INVENTOR(S): Heldmann, Dieter; Stohrer, Juergen; Zauner, Raffael
PATENT ASSIGNEE(S): Consortium Fuer Elektrochemische Industrie GmbH, Germany
SOURCE: Ger. Offen., 10 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

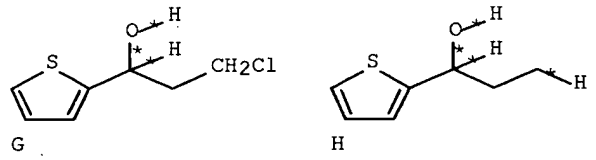
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10248479	A1	20040506	DE 2002-10248479	20021017

PRIORITY APPLN. INFO.: DE 2002-10248479 20021017
OTHER SOURCE(S): MARPAT 140:357198

AB Thienyl-substituted β-haloketones (I; X = Br, Cl) were prepared by reacting thiophene with an acid halide XCH2CH2C(O)Cl (X as above) in the presence of a Friedel-Crafts catalyst selected from organic or inorg. acids, metals, perchlorates, H3PO4 derivs., or halides. The reaction is carried out in such a way that the Friedel-Crafts catalyst is treated with the thiophene and an acid halide. The invention relates as well as preparation of thienyl-substituted secondary aminoalcs. (III; R = alkyl, aralkyl, aryl) by (1) reduction of I to II (X as above), and (2) reacting II with RNH2 (R as above) in a closed system at 0°- 400°. Thus, a suspension of AlCl3 in CH2Cl2 was cooled in an ice bath followed by dropwise treatment with 3-chloropropionyl chloride and subsequently with thiophene at <20°. The reaction mixture was stirred for 1 h at room temperature to give 87% 3-chloro-1-(2-thienyl)-1-propanone. 3-Chloro-1-(2-thienyl)-1-propanol (preparation given) and MeNH2 in THF were heated at 80° for 5 h to give 68% 3-methylamino-1-(2-thienyl)-1-propanol with a purity of >99%.

RX(2) OF 7 ...2 **C** ===> **G** + H...





RX(2) RCT C **40570-64-7**

STAGE(1)
RGT I 16940-66-2 NaBH4, J 1310-73-2 NaOH
SOL 67-63-0 Me2CHOH, 7732-18-5 Water
CON SUBSTAGE(1) room temperature -> -10 deg C
SUBSTAGE(2) -10 deg C -> 10 deg C
SUBSTAGE(3) 2 hours, 10 deg C -> room temperature

STAGE(2)
RGT K 12125-02-9 NH4Cl
SOL 7732-18-5 Water
CON room temperature

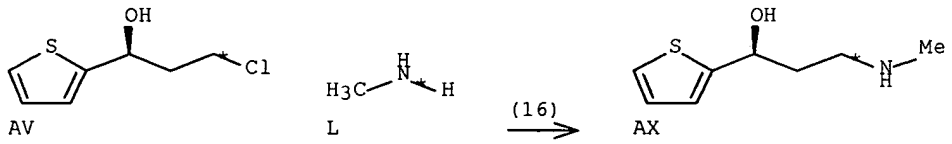
PRO G **260354-12-9**, H 23229-69-8
NTE product ratio is 9:1

IC ICM C07D333-16
ICS C07D333-14
CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
ST chlorothienylpropanone prepn; propanone chloro thienyl prepn; chloropropionyl chloride thiophene Friedel Crafts acylation; methylaminothienylpropanol prepn; propanol methylamino thienyl prepn
IT Acids, uses
RL: CAT (Catalyst use); USES (Uses)
(inorg.; procedure for production of thienyl-substituted secondary aminoalcs.)
IT Acids, uses
RL: CAT (Catalyst use); USES (Uses)
(organic; procedure for production of thienyl-substituted secondary aminoalcs.)
IT Friedel-Crafts reaction catalysts
(procedure for production of thienyl-substituted secondary aminoalcs.)
IT Halides
Metals, uses
Perchlorates
RL: CAT (Catalyst use); USES (Uses)
(procedure for production of thienyl-substituted secondary aminoalcs.)

IT Friedel-Crafts reaction
(procedure for production of thienyl-substituted secondary aminoalcs. by)
IT 23229-69-8P, 1-(2-Thienyl)-1-propanol
RL: BYP (Byproduct); PREP (Preparation)
(procedure for production of thienyl-substituted secondary aminoalcs.)
IT 7446-70-0, Aluminum chloride, uses 7664-38-2D, Phosphoric acid, derivs.
RL: CAT (Catalyst use); USES (Uses)
(procedure for production of thienyl-substituted secondary aminoalcs.)
IT 40570-64-7P, 3-Chloro-1-(2-thienyl)-1-propanone 116539-56-1P, 3-Methylamino-1-(2-thienyl)-1-propanol
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(procedure for production of thienyl-substituted secondary aminoalcs.)
IT 110-02-1, Thiophene 625-36-5, 3-Chloropropionyl chloride 681801-21-8 689262-41-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(procedure for production of thienyl-substituted secondary aminoalcs.)
IT 260354-12-9P, 3-Chloro-1-(2-thienyl)-1-propanol
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(procedure for production of thienyl-substituted secondary aminoalcs.)
IT 116539-55-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(procedure for production of thienyl-substituted secondary aminoalcs.)
IT 50-67-9, Serotonin, biological studies 14838-15-4, Norephedrine
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(uptake inhibitors; procedure for production of thienyl-substituted secondary aminoalcs.)

L46 ANSWER 5 OF 15 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 140:145879 CASREACT Full-text
TITLE: Duloxetine (Cymbalta), a dual inhibitor of serotonin and norepinephrine reuptake
AUTHOR(S): Bymaster, F. P.; Beedle, E. E.; Findlay, J.; Gallagher, P. T.; Krushinski, J. H.; Mitchell, S.; Robertson, D. W.; Thompson, D. C.; Wallace, L.; Wong, D. T.
CORPORATE SOURCE: Eli Lilly and Company, Lilly Research Laboratories, Lilly Corporate Center, Indianapolis, IN, 46285, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(24), 4477-4480
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of naphthalenyloxy-substituted amines I (n = 2 - 4, R = H; n = 1, R = H, Ph, 4-FC6H4, 2-MeOC6H4, 2-furyl, 2-thienyl, 2-thiazolyl, etc.) has been prepared, and these compds. are demonstrated to be inhibitors of both serotonin and norepinephrine reuptake. One member of this series, duloxetine (Cymbalta), (S)-I (n = 1; R = 2-thienyl), has proven to be effective in clin. trials for the treatment of depression.

RX(16) OF 32 ...**AV** + L ===> **AX**...



RX(16) RCT AV **164071-56-1**

STAGE(1)
RGT S 7681-82-5 NaI
SOL 67-64-1 Me2CO

STAGE(2)
RCT L 74-89-5
SOL 109-99-9 THF

PRO AX **116539-55-0**

CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1

ST amine naphthalenyloxy prepn dual inhibitor serotonin norepinephrine reuptake antidepressive; naphthalene aminoalkoxy prepn dual inhibitor serotonin norepinephrine reuptake antidepressive

IT Mental and behavioral disorders
(depression; preparation of naphthalenyloxy-substituted amines as dual inhibitors of serotonin and norepinephrine reuptake and antidepressive agents)

IT 5-HT reuptake inhibitors
Antidepressants
Human
(preparation of naphthalenyloxy-substituted amines as dual inhibitors of serotonin and norepinephrine reuptake and antidepressive agents)

IT 88-15-3, 2-Acetylthiophene 1192-62-7, 2-Acetylfuran 1468-83-3, 3-Acetylthiophene 24295-03-2, 2-Acetylthiazole
RL: RCT (Reactant); RACT (Reactant or reagent)
(Mannich reaction; preparation of naphthalenyloxy-substituted amines as dual inhibitors of serotonin and norepinephrine reuptake and antidepressive agents)

IT 13636-02-7P 116539-55-0P 116817-84-6P 653573-72-9P 653573-73-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(O-arylation; preparation of naphthalenyloxy-substituted amines as dual inhibitors of serotonin and norepinephrine reuptake and antidepressive agents)

IT 164071-56-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(amination; preparation of naphthalenyloxy-substituted amines as dual inhibitors of serotonin and norepinephrine reuptake and antidepressive agents)

IT 63964-28-3P 653573-37-6P 653573-38-7P 653573-39-8P 653573-40-1P 653573-41-2P 653573-42-3P 653573-43-4P 653573-44-5P 653573-45-6P 653573-46-7P 653573-47-8P 653573-48-9P 653573-49-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(demethylation; preparation of naphthalenyloxy-substituted amines as dual inhibitors of serotonin and norepinephrine reuptake and antidepressive agents)

IT 106-93-4, 1,2-Dibromoethane 109-64-8, 1,3-Dibromopropane
110-52-1, 1,4-Dibromobutane 6940-78-9, 1-Bromo-4-chlorobutane
54512-75-3, 1-Bromo-5-chloropentane
RL: RCT (Reactant); RACT (Reactant or reagent)
(naphthol alkylation; preparation of naphthalenyloxy-substituted amines as dual inhibitors of serotonin and norepinephrine reuptake and antidepressive agents)

IT 50-67-9, Serotonin, biological studies 51-41-2, Norepinephrine
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of naphthalenyloxy-substituted amines as dual inhibitors of serotonin and norepinephrine reuptake and antidepressive agents)

IT 50882-69-4P 115600-83-4P 116539-59-4P 116539-60-7P
116817-13-1P 116817-27-7P 116817-39-1P 116817-63-1P
361395-31-5P 653573-30-9P 653573-31-0P 653573-33-2P
653573-34-3P 653573-50-3P 653573-51-4P 653573-52-5P
653573-53-6P 653573-54-7P 653573-55-8P 653573-57-0P
653573-59-2P 653573-61-6P 653573-63-8P 653573-65-0P
653573-67-2P 653573-69-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of naphthalenyloxy-substituted amines as dual inhibitors of serotonin and norepinephrine reuptake and antidepressive agents)

IT 90-15-3, 1-Naphthol 135-19-3, 2-Naphthol, reactions 321-38-0, 1-Fluoronaphthalene
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of naphthalenyloxy-substituted amines as dual inhibitors of serotonin and norepinephrine reuptake and antidepressive agents)

IT 3245-62-3P 3351-50-6P 13247-79-5P 87723-21-5P 164071-55-0P
164071-61-8P 188973-94-6P 653573-32-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of naphthalenyloxy-substituted amines as dual inhibitors of serotonin and norepinephrine reuptake and antidepressive agents)

IT 2138-33-2 2138-34-3 2138-38-7 3506-36-3 13552-47-1
35076-32-5 40570-64-7 46274-54-8 46394-28-9 51949-05-4
55831-59-9 90548-91-7 634924-04-2 653573-35-4 653573-36-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction; preparation of naphthalenyloxy-substituted amines as dual inhibitors of serotonin and norepinephrine reuptake and antidepressive agents)

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 6 OF 15 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 6

ACCESSION NUMBER: 132:207719 CASREACT Full-text

TITLE: Chemo-enzymatic synthesis of the antidepressant duloxetine and its enantiomer

AUTHOR(S): Liu, Huiling; Hoff, Bard Helge; Anthonsen, Thorleif

CORPORATE SOURCE: Department of Chemistry, Norwegian University of Science and Technology, Trondheim, Norway

SOURCE: Chirality (2000), 12(1), 26-29
CODEN: CHRLEP; ISSN: 0899-0042

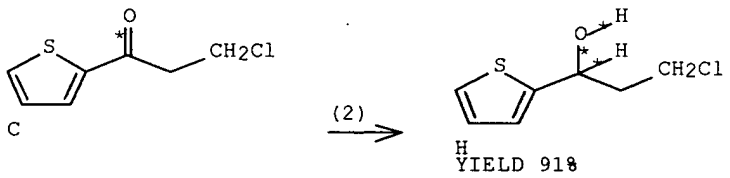
PUBLISHER: Wiley-Liss, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Sodium borohydride reduction of 3-chloro-1-(2-thienyl)-1-propanone gave the corresponding racemic alc., which was kinetically resolved with lipase B from Candida antarctica as catalyst to yield the chiral building blocks (S)-3-chloro-1-(2-thienyl)-1- propanol and the corresponding (R)-butanoate. The enantiopure chiral building blocks were converted to duloxetine and its enantiomer.

RX(2) OF 24 ...C ===> H...



YIELD 91%

RX(2) RCT C **40570-64-7**

STAGE(1)
RGT I 16940-66-2 NaBH4
SOL 64-17-5 EtOH

STAGE(2)
RGT J 12125-02-9 NH4Cl

STAGE(3)
SOL 75-09-2 CH2Cl2

PRO H **260354-12-9**

CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 9

ST duloxetine enantiomer stereoselective prepn; enzymic resoln chlorothienylpropanol intermediate duloxetine; lipase kinetic resoln chlorothienylpropanol

IT Resolution (separation)
(kinetic; of 3-chloro-1-(2-thienyl)-1-propanol by lipase-catalyzed esterification)

IT 164071-55-0P 164071-56-1P
RL: BPN (Biosynthetic preparation); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(chemo-enzymic synthesis of duloxetine and its enantiomer)

IT 260354-14-1P
RL: BPN (Biosynthetic preparation); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(chemo-enzymic synthesis of duloxetine and its enantiomer)

IT 116539-59-4P, Duloxetine 116539-60-7P, (R)-Duloxetine
RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(chemo-enzymic synthesis of duloxetine and its enantiomer)

IT 9001-62-1, Lipase
RL: CAT (Catalyst use); USES (Uses)
(chemo-enzymic synthesis of duloxetine and its enantiomer)

IT 110-02-1, Thiophene 321-38-0, 1-Fluoronaphthalene 625-36-5, 3-Chloropropanoyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(chemo-enzymic synthesis of duloxetine and its enantiomer)

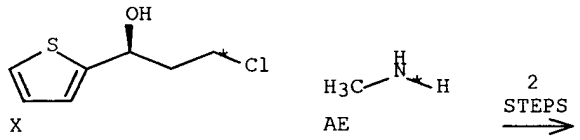
IT 40570-64-7P 116539-55-0P 116539-57-2P 164071-58-3P 260354-12-9P 260354-15-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(chemo-enzymic synthesis of duloxetine and its enantiomer)

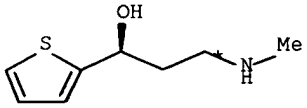
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 7 OF 15 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 7
ACCESSION NUMBER: 123:55626 CASREACT Full-text
TITLE: An asymmetric synthesis of duloxetine hydrochloride, a mixed uptake inhibitor of serotonin and norepinephrine, and its C-14 labeled isotopomers
AUTHOR(S): Wheeler, William J.; Kuo, Fengjiun
CORPORATE SOURCE: Lilly Res. Lab., Eli Lilly Co., Indianapolis, IN, 46285, USA
SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (1995), 36(3), 213-23
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Two 14C-isotopomers of duloxetine HCl [S-(+)-N-methyl-γ-(1- naphthalenyloxy)-2-thiophenepropanamine hydrochloride] have been prepared by an asym. synthesis. The palladium catalyzed cross-coupling of 2-thienoyl chloride (or its [carbonyl-14C] isotopomer) with vinyltributylstannane, followed by addition of HCl afforded the key pro-chiral intermediate chloro ketone. Chiral reduction with borane in the presence of the appropriate oxazaborolidine catalyst provided the S-chloro alc. and its 14C-labeled counterpart or the analogous R-chloro alc. Activation of the chloro alcs. by reaction with NaI/acetone, followed by reaction of the corresponding iodo alcs. with methylamine yielded the penultimate amino alcs. Formation of the alkoxide with NaH, followed by reaction with 1-fluoronaphthalene yielded duloxetine or its 14C-labeled isotopomer. Alternatively, reaction of the R-chloro alc. with 1-naphthol-[1-14C] under Mitsunobu conditions afforded a aryl ether, which was in turn activated by reaction with NaI/acetone. Subsequent reaction with methylamine followed by salt formation yielded duloxetine or its naphthalene-labeled isotopomer as their HCl salts.

RX(30) OF 75 COMPOSED OF RX(9), RX(11)
RX(30) **X** + AE ===> **AF**





AF
YIELD 72%

RX(9) RCT X **164071-56-1**
RGT AB 7681-82-5 NaI
PRO AA 164071-58-3
SOL 67-64-1 Me2CO
NTE in the dark

RX(11) RCT AA 164071-58-3, AE 74-89-5
PRO AF **116539-55-0**
SOL 109-99-9 THF, 7732-18-5 Water
CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 8
ST duloxetine carbon 14 labeled; asym synthesis duloxetine
IT Asymmetric synthesis and induction
(asym. synthesis of duloxetine hydrochloride and its carbon-14 labeled isotopomers)
IT 100306-34-1, Benzenemethanol, α-(2-chloroethyl)-, (S)-
RL: RCT (Reactant); RACT (Reactant or reagent)
(Mitsunobu reaction of chlorophenylpropanol and naphthol)
IT 164071-65-2P 164071-66-3P 164071-67-4P 164071-68-5P
RL: BYP (Byproduct); PREP (Preparation)
(asym. synthesis of duloxetine hydrochloride and its carbon-14 labeled isotopomers)
IT 112022-81-8 112022-83-0
RL: CAT (Catalyst use); USES (Uses)
(asym. synthesis of duloxetine hydrochloride and its carbon-14 labeled isotopomers)
IT 90-15-3, 1-Naphthalenol 321-38-0, 1-Fluoronaphthalene
527-72-0, 2-Thiophenecarboxylic acid 7486-35-3,
Vinyltributylstannane 19481-11-9, 1-Naphthol-1-14C 61714-13-4,
2-Thiophenecarboxylic-14C acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. synthesis of duloxetine hydrochloride and its carbon-14 labeled isotopomers)
IT 13191-29-2P 40570-64-7P 116539-55-0P 164071-53-8P
164071-54-9P 164071-55-0P 164071-56-1P 164071-57-2P
164071-58-3P 164071-59-4P 164071-60-7P 164071-61-8P
164071-62-9P 164071-63-0P 164071-64-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. synthesis of duloxetine hydrochloride and its carbon-14 labeled isotopomers)
IT 116539-59-4P, Duloxetine 136434-34-9P, Duloxetine hydrochloride
164071-50-5P 164071-51-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of duloxetine hydrochloride and its carbon-14 labeled isotopomers)
IT 164071-52-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

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L46 ANSWER 8 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:325360 HCAPLUS Full-text
DOCUMENT NUMBER: 142:392277
TITLE: In situ preparation of chiral compounds derived from oxazaborolidine-borane complexes and their use as catalysts in asymmetric reductions of ketones and ether oximes
INVENTOR(S): Burgos, Alain; Bertrand, Blandine; Frein, Stephane; Pluvie, Jean Francois; Roussiasse, Sonia
PATENT ASSIGNEE(S): PPG-Sipsy, Fr.
SOURCE: Fr. Demande, 30 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

FR 2860794	A1	20050415	FR 2003-11838	2003 1009 <--
FR 2860794	B1	20060203		
FR 2860795	A1	20050415	FR 2004-10701	2004 1011 <--
FR 2860795	B1	20060407		
WO 2005035540	A2	20050421	WO 2004-FR2573	2004 1011 <--
WO 2005035540	A3	20050609		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1673375	A2	20060628	EP 2004-817157	2004 1011 <--
EP 1673375	B1	20070801		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1867571	A	20061122	CN 2004-80029618	2004 1011 <--
JP 2007508280	T	20070405	JP 2006-530431	2004 1011 <--
AT 368672	T	20070815	AT 2004-817157	2004 1011 <--
KR 2007026314	A	20070308	KR 2006-706544	2006 0405 <--
US 2007055068	A1	20070308	US 2006-574871	2006 0406 <--
PRIORITY APPLN. INFO.:			FR 2003-11838 A	2003 1009 <--
			WO 2004-FR2573 W	2004 1011 <--

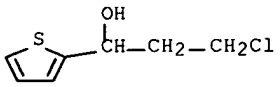
OTHER SOURCE(S): MARPAT 142:392277
ED Entered STN: 15 Apr 2005

AB The invention is related to the in situ preparation of chiral compds. derived from oxazaborolidine-borane complexes by reacting a metal borohydride with a Lewis base, and an ester of an inorg. acid, followed by addition of an optically active amino-alc. and to their use in the preparation of chiral alcs. and ketones by asym. reduction of prochiral ketones and ether oximes. The method eliminates the use of I2 in the preparation of the oxazaborolidine-borane complex. Thus, NaBH4 in THF was mixed with PhNEt2, the mixture cooled to 5°, Me2SO4 added and the mixture stirred at 20° for 1 h, and finally mixed with (R)-diphenylprolinol at 20° for 1 h. A solution of 3-chloro-1-(2-thienyl)propanone in THF was added to the above preheated mixture over a period of 1.5 h, followed by hydrolysis for 1 h at 20° to give the corresponding alc. in high chemical purity.

IT **260354-12-9P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(alc. product; in situ preparation of chiral compds. derived from oxazaborolidine-borane complexes and their use as catalysts in asym. redns. of ketones and ether oximes)

RN 260354-12-9 HCAPLUS

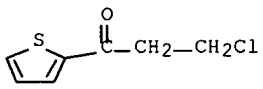
CN 2-Thiophenemethanol, α-(2-chloroethyl)- (CA INDEX NAME)



IT **40570-64-7**, 3-Chloro-1-(2-thienyl)propanone
RL: RCT (Reactant); RACT (Reactant or reagent)
(ketone starting material; in situ preparation of chiral compds. derived from oxazaborolidine-borane complexes and their use as catalysts in asym. redns. of ketones and ether oximes)

RN 40570-64-7 HCAPLUS

CN 1-Propanone, 3-chloro-1-(2-thienyl)- (CA INDEX NAME)



IC ICM C07F005-04

CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 29, 45

IT **260354-12-9P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(alc. product; in situ preparation of chiral compds. derived from oxazaborolidine-borane complexes and their use as catalysts in asym. redns. of ketones and ether oximes)

IT **40570-64-7**, 3-Chloro-1-(2-thienyl)propanone
RL: RCT (Reactant); RACT (Reactant or reagent)
(ketone starting material; in situ preparation of chiral compds. derived from oxazaborolidine-borane complexes and their use as catalysts in asym. redns. of ketones and ether oximes)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 9 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:252497 HCAPLUS Full-text
DOCUMENT NUMBER: 140:287257
TITLE: Process for the preparation of heterocyclic

hydroxypropylamines via amidation and reduction of the corresponding esters.

INVENTOR(S): Houson, Ian Nicholas
PATENT ASSIGNEE(S): Avecia Limited, UK
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004024708	A2	20040325	WO 2003-GB3982	20030912
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WO 2004024708	A3	20040603		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2498756	A1	20040325	CA 2003-2498756	20030912
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AU 2003271844	A1	20040430	AU 2003-271844	20030912
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EP 1542985	A2	20050622	EP 2003-753682	20030912
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CN 1694878	A	20051109	CN 2003-825120	20030912
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JP 2006513145	T	20060420	JP 2004-535693	20030912
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NO 2005001240	A	20050401	NO 2005-1240	20050310
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IN 2005DN00982	A	20070119	IN 2005-DN982	20050314
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US 2005272940	A1	20051208	US 2005-528092	20050316
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PRIORITY APPLN. INFO.: GB 2002-21438 A

2002
0916
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WO 2003-GB3982 W
2003
0912
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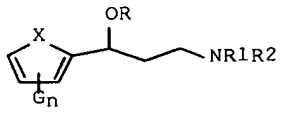
OTHER SOURCE(S): CASREACT 140:287257; MARPAT 140:287257
ED Entered STN: 26 Mar 2004
GI



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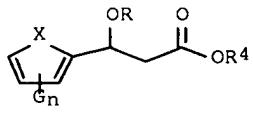


II

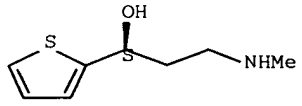
AB Title compds. [I; X = S, O, NR3; R3 = H, organic group; R = H, organic group; R1, R2 = H, (substituted) alkyl, aryl; G = substituent; n = 0-3], were prepared by reaction of ester [II; R4 = (substituted) alkyl, alkenyl, alkynyl, aryl, heteroaryl; other variables as above] with NHR1R2 to give the corresponding amide, followed by reduction Thus, Et (S)-3-hydroxy-3-(2-thienyl)propanoate (preparation given) was stirred 1 h with MeNH2 in PhMe to give 36% (S)-N-Methyl-3-hydroxy-3-(2-thienyl)propanamide. The latter in THF was treated with LiAlH4 in THF to give 88% (S)-3-methylamino-1-(2-thienyl)propan-1-ol.

IT **116539-55-0P**, (S)-3-Methylamino-1-(2-thienyl)propan-1-ol
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of heterocyclic hydroxypropylamines via amidation and reduction of the corresponding esters)

RN 116539-55-0 HCAPLUS

CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

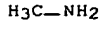
Absolute stereochemistry. Rotation (-).



IT **74-89-5**, Methylamine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of heterocyclic hydroxypropylamines via amidation and reduction of the corresponding esters)

RN 74-89-5 HCAPLUS

CN Methanamine (CA INDEX NAME)



IC ICM C07D333-20
ICS C07D333-22

CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 16

IT **116539-55-0P**, (S)-3-Methylamino-1-(2-thienyl)propan-1-ol
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of heterocyclic hydroxypropylamines via amidation and reduction of the corresponding esters)

IT **74-89-5**, Methylamine, reactions 88-15-3, 2-Acetylthiophene 105-58-8, Diethyl carbonate
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of heterocyclic hydroxypropylamines via amidation and reduction of the corresponding esters)

L46 ANSWER 10 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:120843 HCAPLUS Full-text
DOCUMENT NUMBER: 140:181317
TITLE: Preparation of enantiomerically pure (S)-3-methylamino-1-(thien-2-yl)propan-1-ol from racemic 3-hydroxy-3-(thien-2-yl)propionitrile via kinetic resolution with an acylating agent and a lipase followed by treatment with methylamine and hydrogen in the presence of a catalyst.
INVENTOR(S): Stuermer, Rainer
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004013123	A1	20040212	WO 2003-EP8492	2003 0731
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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CA 2493451	A1	20040212	CA 2003-2493451	2003 0731
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AU 2003251677	A1	20040223	AU 2003-251677	2003 0731
			<--	
EP 1527065	A1	20050504	EP 2003-766383	2003 0731
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EP 1527065	B1	20061122		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,				

	MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
CN 1671687	A	20050921	CN 2003-818510	2003 0731 <--
JP 2006507234	T	20060302	JP 2004-525403	2003 0731 <--
AT 346061	T	20061215	AT 2003-766383	2003 0731 <--
ES 2278203	T3	20070801	ES 2003-3766383	2003 0731 <--
US 2005245749	A1	20051103	US 2005-522888	2005 0624 <--
PRIORITY APPLN. INFO.:			DE 2002-10235206 A	2002 0801 <--
			WO 2003-EP8492 W	2003 0731 <--

OTHER SOURCE(S): CASREACT 140:181317

ED Entered STN: 13 Feb 2004

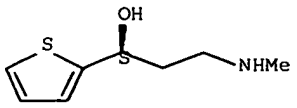
AB A process for the preparation of enantiomerically pure (S)-3-methylamino-1-(thien-2-yl)propan-1-ol (I) comprises treatment of of a mixture of (R)- and (S)-3-hydroxy-3-thien-2- ylpropionitrile with an acylating agent in the presence of a hydrolase to give a mixture of unacylated (S)-3-hydroxy-3-thien-2- ylpropionitrile and acylated (R)-nitrile and treatment of the former with hydrogen and methylamine in the presence of a catalyst. Thus, 3-hydroxy-3-thien-2-ylpropionitrile (preparation given) was shaken with lipase from Pseudomonas DSM 8246 and vinyl hexanoate in Me tert-Bu ether for 6 h at room temperature to give after flash chromatog. 48% (S)-3-hydroxy-3-thien-2-ylpropionitrile in 99.4% enantiomeric excess. The latter was autoclaved with MeNH2 in MeOH over Raney Ni under 50 bar H2 at 65° for 24 h to give 79% I.

IT **116539-55-0P**, (S)-3-Methylamino-1-(thien-2-yl)propan-1-ol
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropionitrile via kinetic resolution followed by catalytic reductive amination with methylamine)

RN 116539-55-0 HCAPLUS

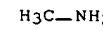
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT **74-89-5**, Methylamine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropionitrile via kinetic resolution

followed by catalytic reductive amination with methylamine)
RN 74-89-5 HCAPLUS
CN Methanamine (CA INDEX NAME)



IC ICM C07D333-20
ICS C07B057-00
CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 7
IT **116539-55-0P**, (S)-3-Methylamino-1-(thien-2-yl)propan-1-ol
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropionitrile via kinetic resolution followed by catalytic reductive amination with methylamine)
IT **74-89-5**, Methylamine, reactions 75-05-8, Acetonitrile, reactions 98-03-3, Thiophene-2-carboxaldehyde 105-38-4, Vinyl propionate 108-30-5, Succinic anhydride, reactions 3050-69-9, Vinyl hexanoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropionitrile via kinetic resolution followed by catalytic reductive amination with methylamine)

L46 ANSWER 11 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:286808 HCAPLUS Full-text
DOCUMENT NUMBER: 140:302436
TITLE: Process for the production of 3-heteroaryl-3-hydroxy-propionic acid derivatives by enantioselective microbial reduction
INVENTOR(S): Berendes, Frank; Eckert, Markus; Brinkmann, Nils; Dreisbach, Claus; Meissner, Ruth; Koch, Rainhard
PATENT ASSIGNEE(S): Bayer Chemicals A.-G., Germany
SOURCE: Eur. Pat. Appl., 16 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

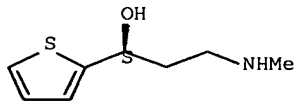
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1405917	A2	20040407	EP 2003-20847	2003 0913 <--
EP 1405917	A3	20050112		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
DE 10244811	A1	20040408	DE 2002-10244811	2002 0926 <--
IN 2003MU00922	A	20050715	IN 2003-MU922	2003 0908 <--

US 2004181058	A1	20040916	US 2003-669424	2003 0924 <--
JP 2004113245	A	20040415	JP 2003-335690	2003 0926 <--
CN 1497048	A	20040519	CN 2003-160307	2003 0926 <--
US 2006264641	A1	20061123	US 2006-436347	2006 0518 <--

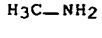
PRIORITY APPLN. INFO.: DE 2002-10244811 A 2002 0926 <--
US 2003-669424 A3 2003 0924 <--

OTHER SOURCE(S): MARPAT 140:302436
ED Entered STN: 08 Apr 2004
AB A process for the production of 3-heteroaryl-3-hydroxy-propionic acid derivs. by enantioselective microbial reduction is provided. Thus, Saccharomyces cerevisiae was used to reduce methyl-3-oxo-3-(2- thiophenyl)propanoic acid to methyl-(3S)-hydroxy-3-(2- thiophenyl)propanoic acid with a yield of 75% and an enantiomeric excess >97%. The reaction product then served as a reactant in the chemical synthesis of (1S)-3-(methylamino)-1-(2-thienyl)-1- propanol.
IT **116539-55-0P**
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(process for production of 3-heteroaryl-3-hydroxy-propionic acid derivs. by enantioselective microbial reduction)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT **74-89-5**, Methylamine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for production of 3-heteroaryl-3-hydroxy-propionic acid derivs. by enantioselective microbial reduction)
RN 74-89-5 HCAPLUS
CN Methanamine (CA INDEX NAME)



IC ICM C12P017-00
ICS C12P041-00; C07D213-55; C07D213-56; C07D333-24; C07D333-60;

C07D307-54
CC 16-5 (Fermentation and Bioindustrial Chemistry)
IT **116539-55-0P** 116539-57-2P, (1R)-3-(Methylamino)-1-(2-thienyl)-1-propanol 116539-59-4P 116539-60-7P 121776-72-5P, (S)-3-Hydroxy-3-(2-furanyl)propanenitrile 129101-56-0P, (S)-Ethyl 3-hydroxy-3-(2-furanyl)propanoate 132335-44-5P, (1S)-3-(Dimethylamino)-1-(2-thienyl)-1-propanol 132335-49-0P, (1R)-3-(Dimethylamino)-1-(2-thienyl)-1-propanol 238093-29-3P, (S)-Methyl 3-hydroxy-3-(2-thienyl)propanoate 477722-37-5P, (S)-Methyl 3-hydroxy-3-(2-furanyl)propanoate 503188-05-4P, (S)-3-Hydroxy-3-(3-pyridinyl)propanenitrile 591727-36-5P, (S)-3-Hydroxy-3-(2-thienyl)propanenitrile 603959-56-4P, (S)-3-Hydroxy-3-(2-thienyl)propanoic acid N-methylamide 666740-61-0P, (S)-Methyl 3-hydroxy-3-(3-furanyl)propanoate 666740-62-1P, (S)-Methyl 3-hydroxy-3-(3-thienyl)propanoate 676563-08-9P, (S)-Ethyl 3-hydroxy-3-(3-thienyl)propanoate 676563-09-0P, (S)-Ethyl 3-hydroxy-3-(3-furanyl)propanoate 676563-10-3P, (S)-Methyl 3-hydroxy-3-(2-pyridinyl)propanoate 676563-11-4P, (S)-Ethyl 3-hydroxy-3-(2-pyridinyl)propanoate 676563-12-5P, (S)-Methyl 3-hydroxy-3-(3-pyridinyl)propanoate 676563-13-6P, (S)-Ethyl 3-hydroxy-3-(3-pyridinyl)propanoate 676563-14-7P, (S)-Methyl 3-hydroxy-3-(4-pyridinyl)propanoate 676563-15-8P, (S)-Ethyl 3-hydroxy-3-(4-pyridinyl)propanoate 676563-16-9P, (S)-3-Hydroxy-3-(3-thienyl)propanenitrile 676563-17-0P, (S)-3-Hydroxy-3-(3-furanyl)propanenitrile 676563-18-1P, (S)-3-Hydroxy-3-(2-pyridinyl)propanenitrile 676563-19-2P, (S)-3-Hydroxy-3-(4-pyridinyl)propanenitrile 676596-56-8P 676596-57-9P
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(process for production of 3-heteroaryl-3-hydroxy-propionic acid derivs. by enantioselective microbial reduction)
IT **74-89-5**, Methylamine, reactions 88-15-3, 2-ACetylthiophene 616-38-6, Dimethyl carbonate 7784-21-6, Aluminum hydride 13283-31-3, Boron hydride, reactions 16853-85-3, Lithium aluminum hydride
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for production of 3-heteroaryl-3-hydroxy-propionic acid derivs. by enantioselective microbial reduction)

L46 ANSWER 12 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:605494 HCAPLUS Full-text
DOCUMENT NUMBER: 141:140312
TITLE: 3-Methylamino-1-(2-thienyl)-1-propanone preparation and its use as a pharmaceutical intermediate
PATENT ASSIGNEE(S): BASF Ag, Germany
SOURCE: Ger. Offen., 4 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10302595	A1	20040729	DE 2003-10302595 <--	2003 0122
CA 2513542	A1	20040805	CA 2004-2513542 <--	2004 0115
WO 2004065376	A1	20040805	WO 2004-EP237	2004

0115

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EP 1587802 A1 20051026 EP 2004-702333
2004
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EP 1587802 B1 20071114
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CN 1742003 A 20060301 CN 2004-80002686
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JP 2006515878 T 20060608 JP 2006-500570
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AT 378326 T 20071115 AT 2004-702333
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US 2006128791 A1 20060615 US 2005-542003
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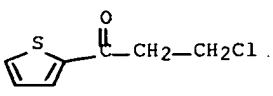
ED Entered STN: 29 Jul 2004

AB 3-Methylamino-1-(2-thienyl)-1-propanone and its acid addition salts (e.g., the hydrochloride), which are useful as an intermediate in the production of the pharmaceutical (+)-(S)-N-methyl-3-(1- naphthyloxy)-3-(2-thienyl)propylamine oxalate (i.e., Duloxetine oxalate), are prepared

IT **40570-64-7**, 3-Chloro-1-(2-thienyl)-1-propanone
RL: RCT (Reactant); RACT (Reactant or reagent)
(in the preparation of 3-methylamino-1-(2-thienyl)-1-propanone)

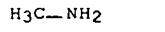
RN 40570-64-7 HCAPLUS

CN 1-Propanone, 3-chloro-1-(2-thienyl)- (CA INDEX NAME)



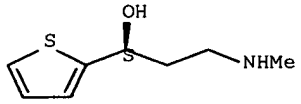
IT **74-89-5**, Methylamine, reactions
RL: RCT (Reactant); RGT (Reagent); RACT (Reactant or reagent)
(in the preparation of 3-methylamino-1-(2-thienyl)-1-propanone)

RN 74-89-5 HCAPLUS
CN Methanamine (CA INDEX NAME)



IT **116539-55-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)-
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IC ICM C07D333-20
ICS C07D333-10; C12P017-00
CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
IT 5424-47-5 **40570-64-7**, 3-Chloro-1-(2-thienyl)-1-propanone
494221-37-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(in the preparation of 3-methylamino-1-(2-thienyl)-1-propanone)
IT **74-89-5**, Methylamine, reactions
RL: RCT (Reactant); RGT (Reagent); RACT (Reactant or reagent)
(in the preparation of 3-methylamino-1-(2-thienyl)-1-propanone)
IT **116539-55-0P** 116539-56-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L46 ANSWER 13 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:198151 HCAPLUS Full-text
DOCUMENT NUMBER: 140:253344
TITLE: Preparation of (3R) - or (3S)-3-oxy-3-(2-thiophen)propylamines and related compounds via an enantioselective Reformatskii reaction
INVENTOR(S): Sorger, Klas; Stratmann, Oliver; Petersen, Hermann; Stohrer, Juergen
PATENT ASSIGNEE(S): Consortium fuer Elektrochemische Industrie G.m.b.H., Germany
SOURCE: Ger. Offen., 29 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10237272	A1	20040311	DE 2002-10237272 <--	20020814
PRIORITY APPLN. INFO.:			DE 2002-10237272	20020814

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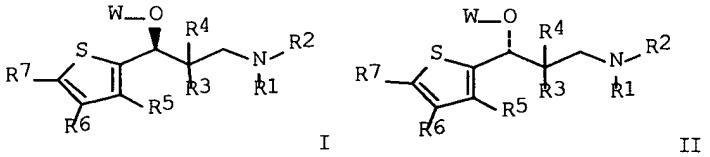
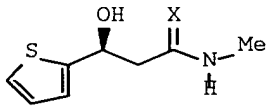
OTHER SOURCE(S): MARPAT 140:253344
ED Entered STN: 11 Mar 2004
GI



I II

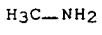


III

AB Title compds. I and II [R1, R2 = H, halo-alkyl, CN-alkyl; R3, R4, R5, R6, R7 = H, halo, halo-alkyl; W = H, alkyl, acyl, etc.] were prepared via a sparteine mediated enantioselective Reformatskii reaction. For example, LAH reaction of amide II (X = O), e.g., prepared from 2-thiophenecarboxaldehyde in 2-steps, afforded propylamine in 90% yield and 89% ee (HPLC).

IT **74-89-5**, Methylamine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (3S)-3-oxy-3-(2-thiophen)propylamines and related compds. via an enantioselective Reformatskii reaction)

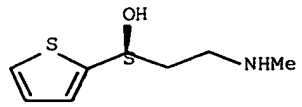
RN 74-89-5 HCAPLUS
CN Methanamine (CA INDEX NAME)



IT **116539-55-0P**, N-Methyl-(S)-(-)-3-Hydroxy-3-(2-thiophen)propylamine
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (3S)-3-oxy-3-(2-thiophen)propylamines and related compds. via an enantioselective Reformatskii reaction)

RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IC ICM C07D333-04
ICS C07D333-06; A61K031-381

CC 25-17 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 21

IT 74-88-4, Methyliodide, reactions **74-89-5**, Methylamine, reactions 75-36-5, Acetyl chloride 75-77-4, Trimethylchlorosilane, reactions 96-32-2, Bromoacetic acid methyl ester 98-03-3, 2-Thiophenecarboxaldehyde 105-36-2, Bromoacetic acid ethyl ester 590-17-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (3S)-3-oxy-3-(2-thiophen)propylamines and related compds. via an enantioselective Reformatskii reaction)

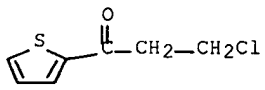
IT **116539-55-0P**, N-Methyl-(S)-(-)-3-Hydroxy-3-(2-thiophen)propylamine 591727-36-5P, (S)-(-)-3-Hydroxy-3-(2-thiophen)propane nitrile 603959-54-2P, (S)-(-)-3-Hydroxy-3-(2-thiophen)propionic acid ethyl ester 666740-52-9P, (S)-(-)-3-Methoxy-3-(2-thiophen)propionic acid methyl ester 666740-53-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (3S)-3-oxy-3-(2-thiophen)propylamines and related compds. via an enantioselective Reformatskii reaction)

L46 ANSWER 14 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:525413 HCAPLUS Full-text
DOCUMENT NUMBER: 139:85232
TITLE: Preparation of optically active thienylpropanols
INVENTOR(S): Ogura, Kuniyoshi; Mori, Hiroyuki; Inoue, Yoshiki
PATENT ASSIGNEE(S): Mitsubishi Rayon Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003192681	A	20030709	JP 2001-397944	2001 1227 <--

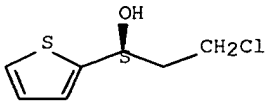
PRIORITY APPLN. INFO.: JP 2001-397944 2001 1227 <--

ED Entered STN: 10 Jul 2003
AB (S)-3-N-methylamino-1-(2-thienyl)-1-propanol is prepared by reaction of thiophene with 3-chloropropionyl chloride in the presence of Friedel-Crafts catalysts, hydrogenation of 1-(2-thienyl)-3- chloropropan-1-one (I) in the presence of transition metal-containing asym. hydrogenation catalysts, bases, and optically active N compds., and reaction of (S)-3-chloro-1-(2-thienyl)-1-propanol (II) with MeNH2. I was hydrogenated in 2-propanol in the presence of KOH, (R,R)-diphenylethylenediamine, and RuCl2[(R)-BINAP](DMF)n at 28° for 6 h to give ≥99% II with 97% ee.
IT **40570-64-7P 164071-56-1P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of optically active thienylpropanols via asym. hydrogenation of thienylchloropropanone)
RN 40570-64-7 HCAPLUS
CN 1-Propanone, 3-chloro-1-(2-thienyl)- (CA INDEX NAME)



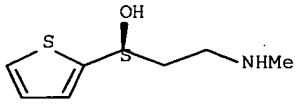
RN 164071-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-(2-chloroethyl)-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT **116539-55-0P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of optically active thienylpropanols via asym. hydrogenation of thienylchloropropanone)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IC ICM C07D333-02
ICS C07B061-00; C07M007-00
CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
IT **40570-64-7P 164071-56-1P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of optically active thienylpropanols via asym. hydrogenation of thienylchloropropanone)
IT **116539-55-0P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of optically active thienylpropanols via asym. hydrogenation of thienylchloropropanone)

L46 ANSWER 15 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:752682 HCAPLUS Full-text
DOCUMENT NUMBER: 139:261162
TITLE: Preparation of arylaminopropanols via ruthenium mediated enantioselective reduction of β-hydroxy esters
INVENTOR(S): Eckert, Markus; Dreisbach, Claus; Bosch, Boris; Stolle, Andreas
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany
SOURCE: Eur. Pat. Appl., 24 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1346977	A1	20030924	EP 2003-4920	2003 0307
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DE 10212301	A1	20031002	DE 2002-10212301	2002 0320
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US 2003225153	A1	20031204	US 2003-391348	2003 0318
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US 7169938	B2	20070130		
CN 1445224	A	20031001	CN 2003-107316	2003 0320
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JP 2003313184	A	20031106	JP 2003-78367	2003 0320
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PRIORITY APPLN. INFO.: DE 2002-10212301 A 2002 0320
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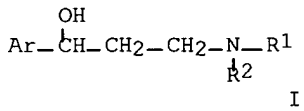
OTHER SOURCE(S): CASREACT 139:261162; MARPAT 139:261162
ED Entered STN: 25 Sep 2003
GI



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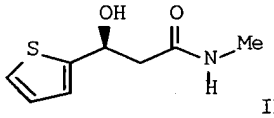

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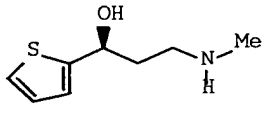


III

AB Title compds. I [Ar = (un)substituted aryl; R1, R2 = H, alkyl, aryl, etc.] were prepared For example, LAH reduction of amide II, e.g., prepared from 2-acetylthiophene in 3-steps, afforded aminopropanol III in 84% yield. Compds. I are claimed useful intermediates for the production of pharmaceuticals.

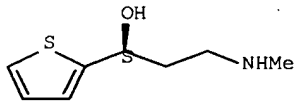
IT **74-89-5**, Methylamine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of arylaminopropanols via ruthenium mediated enantioselective reduction of β-hydroxy esters)

RN 74-89-5 HCAPLUS
CN Methanamine (CA INDEX NAME)

H_3C-NH_2

IT **116539-55-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(product; preparation of arylaminopropanols via ruthenium mediated enantioselective reduction of β-hydroxy esters)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)-
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IC ICM C07C213-00
ICS C07C231-18; C07C051-347; C07C067-00; C07C215-30; C07C235-34; C07C059-48; C07C069-732; C07D333-20
CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
IT **74-89-5**, Methylamine, reactions 88-15-3, 2-Acetylthiophene 94-02-0, Ethyl-3-oxo-3-(phenyl)propanoate 614-27-7, Methyl-3-oxo-3-(phenyl)propanoate 616-38-6, Dimethylcarbonate 13669-10-8 22027-51-6 27835-00-3 54441-65-5 54441-66-6 122334-39-8 612841-65-3 612841-67-5 612841-86-8 612841-92-6, 2-Ethylhexyl-3-oxo-3-(4-tolyl)propanoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of arylaminopropanols via ruthenium mediated enantioselective reduction of β-hydroxy esters)
IT **116539-55-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(product; preparation of arylaminopropanols via ruthenium mediated enantioselective reduction of β-hydroxy esters)
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

FULL SEARCH HISTORY

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                D ALL
                SEL RN

     FILE 'REGISTRY' ENTERED AT 15:07:39 ON 03 JAN 2008
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                116539-55-0/BI OR 142-82-5/BI OR 164071-56-1/BI OR
                16940-66-2/BI OR 23229-69-8/BI OR 260354-12-9/BI OR
                40570-64-7/BI OR 74-89-5/BI OR 861995-99-5/BI OR
                9001-62-1/BI OR 96-49-1/BI)
                D SCAN
L3            6 SEA ABB=ON  PLU=ON  L2 AND 1/S
                D SCAN
L4            7 SEA ABB=ON  PLU=ON  L2 NOT L3
                D SCAN
                D L3 1-6
L5            1 SEA ABB=ON  PLU=ON  40570-64-7/RN
                D SCAN
L6            1 SEA ABB=ON  PLU=ON  116539-55-0/RN
                D SCAN
L7            1 SEA ABB=ON  PLU=ON  260354-12-9/RN
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     FILE 'REGISTRY' ENTERED AT 15:17:42 ON 03 JAN 2008
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L9            1 SEA ABB=ON  PLU=ON  861995-99-5/RN
L10           1 SEA ABB=ON  PLU=ON  L2 AND C4 H4 O3/MF
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L11           1 SEA ABB=ON  PLU=ON  108-30-5/RN
                D SCAN L4
L12           1 SEA ABB=ON  PLU=ON  METHANAMINE/CN
                D RN
L13           1 SEA ABB=ON  PLU=ON  L2 AND LIPASE
                D CN
                D RN
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                D SCAN
L16           4 SEA ABB=ON  PLU=ON  L5/RCT(L)L7/PRO
                D SCAN
L17           2 SEA ABB=ON  PLU=ON  L7/RCT(L)L8/PRO
                D SCAN
L18           4 SEA ABB=ON  PLU=ON  L8/RCT(L)L6/PRO
                D SCAN
L19           7 SEA ABB=ON  PLU=ON  (L15 OR L16 OR L17 OR L18)
                SAV L19 CHA440CRCT/A

     FILE 'STNGUIDE' ENTERED AT 15:44:09 ON 03 JAN 2008

     FILE 'HCAPLUS' ENTERED AT 15:46:30 ON 03 JAN 2008
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                E STUERMER R/AU
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                D SCAN L1
L21             QUE ABB=ON  PLU=ON  CHIRAL? OR ENANTIOMER? OR RESOLUTIO
                N?
L22          35 SEA ABB=ON  PLU=ON  L20 AND L21
L23             QUE ABB=ON  PLU=ON  PY<2005 OR PRY<2005 OR AY<2005 OR
                MY<2005 OR REVIEW/DT
L24          31 SEA ABB=ON  PLU=ON  L22 AND L23
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L30           9 SEA ABB=ON  PLU=ON  L28 AND L29
                D SCAN
L31           7 SEA ABB=ON  PLU=ON  L7
L32           5 SEA ABB=ON  PLU=ON  L28 AND L31
L33           9 SEA ABB=ON  PLU=ON  L8
L34           1 SEA ABB=ON  PLU=ON  L9
L35       11297 SEA ABB=ON  PLU=ON  L11
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L37           2 SEA ABB=ON  PLU=ON  L31 AND ((L33 OR L34 OR L35 OR
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L38           5 SEA ABB=ON  PLU=ON  ((L33 OR L34)) AND L29
L39       19367 SEA ABB=ON  PLU=ON  L12
L40           1 SEA ABB=ON  PLU=ON  L38 AND L39
L41           8 SEA ABB=ON  PLU=ON  (L33 OR L34 OR L29) AND L39
                D SCAN
L42          10 SEA ABB=ON  PLU=ON  L30 OR L32 OR L37 OR L38 OR L40
L43          15 SEA ABB=ON  PLU=ON  L42 OR L41
L44          15 SEA ABB=ON  PLU=ON  L43 AND L23
                D SCAN
                SAV TEMP L44 CHA440HCP/A

     FILE 'STNGUIDE' ENTERED AT 16:02:51 ON 03 JAN 2008
                D QUE L27
                D QUE L24

     FILE 'CASREACT, HCAPLUS' ENTERED AT 16:04:00 ON 03 JAN 2008
L45          30 DUP REM L27 L24 (17 DUPLICATES REMOVED)
                     ANSWERS '1-16' FROM FILE CASREACT
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                D L45 1-30 IBIB ED
                D QUE L19
                D QUE STAT L44
L46          15 DUP REM L19 L44 (7 DUPLICATES REMOVED)
                     ANSWERS '1-7' FROM FILE CASREACT
                     ANSWERS '8-15' FROM FILE HCAPLUS
                D L46 1-7 IBIB AB FHIT IND
                D L46 8-15 IBIB ED ABS HITSTR HITIND
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